# ASSESSMENT OF CONTAMINATION FROM LEAKS OF HAZARDOUS MATERIALS IN THE SANTA CLARA GROUNDWATER BASIN

## 205j REPORT

## Technical Appendix: Chemical Summaries

Cooperative Report By:
San Francisco Regional Water
Quality Control Board
SEEHRL, University of
California, Berkeley
Santa Clara Valley Water District

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# IN THE
# SANTA CLARA GROUNDWATER BASIN

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## TECHNICAL APPENDIX: CHEMICAL SUMMARIES

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# TABLE OF CONTENTS

I. INTRODUCTION....................................................1

II. CHEMICAL SUMMARIES....................................8

III. MUTAGENICITY DATA ABBREVIATIONS......................69

IV. REFERENCES....................................................72

# I. INTRODUCTION

A list of the most frequently found synthetic organic compounds is shown in Table 1. The majority of the compounds are considered volatile organic compounds (VOCs). Chemical summaries including the following information were compiled for each of the chemicals listed in Table 1.

-Synonyms and structure,

-Physical properties: molecular weight, boiling point, vapor pressure, solubility, octanol-water coefficient, and sorption coefficient,

-Uses of chemical, and environmental fate,

-Toxicity: general harmful effects, oral and dermal exposure data, aquatic data, carcinogenicity data, mutagenicity and reproductive data, and

-Federal and State drinking water standards.

These summaries are contained in Section II of this Appendix.

The references used to compile this information include the Environmental Protection Agency's (EPA) ambient water quality criteria documents, EPA's "Water-Related Environmental Fate of 129 Priority Pollutants", and the "Handbook of Environmental Data on Organic Chemicals". Citations for these and other references used to compile this data are contained in Section IV of this Appendix. In addition to the manual methods of literature review, the Registry of Toxic Effects of Chemical Substances (RTECS) and the Toxicological Data Bank (TDB) computer data bases were used to retrieve relevant information.

The scales, as shown in Table 2, used to rate the contaminants were adapted from the work of the Michigan Department of Natural Resources (18) and follow generally accepted terminology. Data for each route of acute toxicity exposure is scored independently, and the highest score of the three routes is used, giving the most conservative estimate of risk. Carcinogenicity determination follows the International Agency for Research on Cancer (IARC) classifications, and mutagenicity ranking reflects positive mutation test results cited in the Registry of Toxic Effects of Chemical Substances (RTECS). Definitions for the RTECS mutagenicity data abbreviations are contained in Section III.

Values for soil sorption (Log Ksc) and bioaccumulation (Log Kow) were obtained directly from the literature by replacing descriptive ratings (low-high) which appear in the work of Swann *et al.* (19) for soil sorption and the Michigan Department of Natural Resources for bioaccumulation, with numerical rankings (0-10). The scales used for these parameters are shown in Table 3.

A summary of the scoring for those compounds used in the site ranking process is shown in Table 4. Review of this Table indicates that, in general, data for all factors except dermal LD50 toxicity data and carcinogenicity data were available and uncertainty was limited. The high degree of uncertainty associated with the dermal LD50 and carcinogenicity factors was due to the general lack of data.

# TABLE 1

## 20 Most Frequently Found Contaminants

| Contaminant | Number Of Sites With Contaminant |
|---|---|
| 1,1,1-Trichloroethane | 64 |
| Trichloroethylene | 60 |
| Trichlorofluoromethane | 53 |
| Tetrachloroethene | 49 |
| Xylene | 47 |
| 1,2-Dichloroethylene | 44 |
| Toluene | 44 |
| Trichloromethane | 41 |
| 1,1-Dichloroethane | 39 |
| 1,1-Dichloroethylene | 39 |
| Ethyl benzene | 36 |
| Methylene chloride | 33 |
| Acetone | 29 |
| Benzene | 27 |
| Isopropyl alcohol | 20 |
| Methyl ethyl ketone | 17 |
| Vinyl chloride | 15 |
| Phthalate esters | 14 |
| 1,2,4-Trichlorobenzene | 12 |
| Phenol | 10 |

# TABLE 2

## Toxicity Scales

### Scale 15 Acute Toxicity

| Score | Category<br>Oral LD50<br>mg/kg | <br>Dermal LD50<br>mg/kg | <br>Aquatic LC50<br>mg/L |
|---|---|---|---|
| 10 | 5 | 5 | 1 |
| 5 | 5-50 | 5-200 | 1-10 |
| 3 | 50-500 | 200-500 | 10-100 |
| 1 | 500-5000 | 500-5000 | 100-1000 |
| 0 | 5000 | 5000 | 1000 |
| 0-10 | Insufficient information | | |

### Scale 16 Carcinogenicity

| Score | Category |
|---|---|
| 10 | Human positive; Human suspect; Animal positive |
| 5 | Animal suspect |
| 0 | Not a known carcinogen |
| 0-10 | Insufficient information |

### Scale 17 Mutagenicity

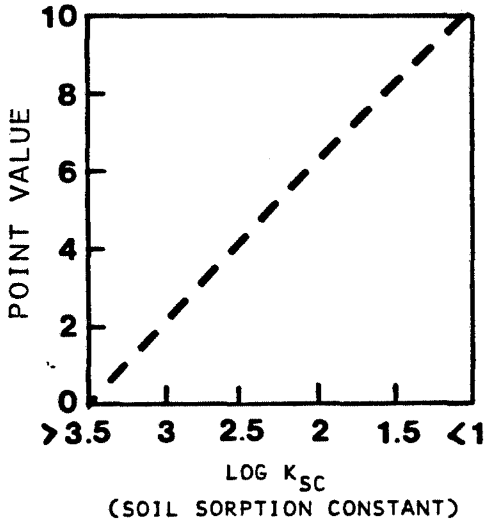
| Score | Category |
|---|---|
| 10 | Positive in multicellular and microorganisms |
| 6 | Positive in multicellular organisms |
| 3 | Positive in microorganisms |
| 0 | Not a known mutagen |
| 0-10 | Insufficient information |

## TABLE 3

## Soil Sorption and Bioaccumulation Scales

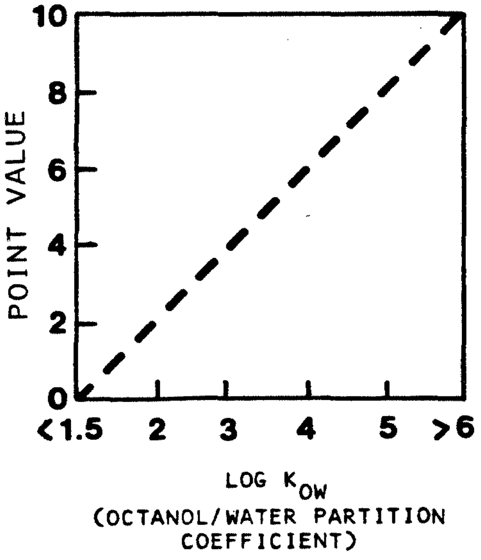
SCALE 18

SOIL SORPTION



SCALE 19

BIOACCUMULATION



# TABLE 4

## Severity Ranking Scores For 20 Most Frequently Found Contaminants

| Contaminant | Acute Toxicity | | | Chronic Toxicity | | Parameters | |
|---|---|---|---|---|---|---|---|
| | O-LD50 | D-LD50 | A-LC50 | Carc | Mutag | Ksc | Kow |
| 1,1,1-Trichloroethane (TCA) | 1 | 0-10 | 3 | 0-10 | 10 | 4-5 | 2-3 |
| Trichloroethylene (TCE) | 1 | 0-10 | 3 | 10b | 10 | 4.5 | 2 |
| Trichlorofluoromethane (Freon) | 0-10 | 0-10 | 0-10 | 0-10 | 0-10 | 4 | 3 |
| Tetrachloroethene (PCE) | 0 | 0-10 | 3 | 10b | 10 | 4 | 3 |
| Xylene | 1 | 0 | 3 | 0-10 | 3 | 1-3.5 | 3.5-4 |
| 1,2-Dichloroethylene (DCE) | 1 | 0-10 | 1 | 0-10 | 0-10 | 8 | 0 |
| Toluene | 1 | 0 | 3 | 0-10 | 10 | 3.5 | 3.5 |
| Trichloromethane (Chloroform) | 5 | 0-10 | 3 | 10a | 10 | 6 | 2 |
| 1,1-Dichloroethane (DCA) | 1 | 0-10 | 0-10 | 0-10 | 0 | 7 | 1 |
| 1,1-Dichloroethylene (DCE) | 3 | 0-10 | 1 | 10b | 3-10 | 8-10 | 0 |
| Ethyl benzene | 1 | 1 | 3 | 0-10 | 0-10 | 1.5 | 4 |
| Methylene chloride | 1 | 0-10 | 1 | 0-10 | 10 | 9 | 0 |
| Acetone | 1 | 0 | 0 | 0-10 | 3 | 10 | 0 |
| Benzene | 1 | 0-10 | 3 | 10c | 10 | 6 | 2 |
| Isopropyl alcohol (IPA) | 0 | 0 | 1 | 10a | 10 | 10 | 0 |
| Methyl ethyl ketone (MEK) | 1 | 0 | 0 | 0-10 | 0-10 | 10 | 0 |
| Vinyl chloride | 3 | 0-10 | 3 | 10c | 10 | 10 | 0 |

## TABLE 4 con't

| Contaminant | Acute Toxicity |  |  | Chronic Toxicity |  | Parameters |  |
|---|---|---|---|---|---|---|---|
|  | O-LD50 | D-LD50 | A-LC50 | Carc | Mutag | Ksc | Kow |
| Phthalate esters * | 1 | 0 | 10 | 10b | 10 | 0-5.5 | 2-10 |
| 1,2,4-Trichlorobenzene (TCB) | 3 | 0-10 | 5 | 0-10 | 0-10 | 0 | 6.5 |
| Phenol | 3 | 1 | 3 | 0 | 10 | 8 | 0 |

Note:
The higher the number, the greater the severity score.
A range 0-10 indicates complete uncertainty.

Legend:
Acute Toxicity
LD50 = Dose of chemical needed to produce death in 50 % of the exposed animals
LC50 = Concentration of chemical in water needed to produce death in 50 % of exposed aquatic organisms
O-LD50 = Oral Lethal Dose 50
D-LD50 = Dermal Lethal Dose 50
A-LC50 = Aquatic Lethal Concentration 50, 96-hour test
Chronic Toxicity
Carc = Carcinogenicity
10a = Human Suspect
10b = Animal Positive
10c = Human Positive
Mutag = Mutagenicity
Parameters
Log Ksc = Soil Sorption Coefficient
Log Kow = Octanol-Water Coefficient

* Phthalate esters = Dimethyl, Diethyl, Di-n-butyl, Di-n-octyl, Bis(2-ethylhexyl), and Butyl benzyl phthalates

# II. CHEMICAL SUMMARIES

# ACETONE

File Name: B:Acetone
NIOSH# AL3150000

## I. CHEMICAL INFORMATION

Synonyms (10):
- Dimethylformaldehyde
- Dimethyl Ketal
- Dimethyl Ketone
- Ketone Propane
- Methyl Ketone
- Propanone
- 2-Propanone
- Pyroacetic Acid
- Pyroacetic Ether
- Beta-Ketopropane

Structure:

$CH_3-CO-CH_3$

Physical Properties (9 except where noted):

Mol. Wt.: 58.08
Melting Pt.: -94 C
Boiling Pt.: 56.5 C
Vapor Pressure: 185 mm at 25 C (3)

Solubility: infinite (3)
Kow: -0.24 (15)
Ksc: ~ -0.24

Uses (3):

Acetone is used as a solvent, in the production of lubricating oils and as an intermediate in the manufacture of chloroform and of various pharmaceuticals and pesticides. (H)

Detection:

insufficient information

Fate in the Environment:

Volatilization: insufficient information
Photolysis: insufficient information
Sorption: insufficient information
Oxidation: In aerated aqueous systems, acetone is thought to be stripped easily (3).
Hydrolysis: see Oxidation
Bioaccumulation: insufficient information
Biotransformation/Biodegradation: Acetone is assumed to be readily degraded by bacteria (3).

## II. TOXICITY INFORMATION (3 except where noted)

In humans the effects of acetone are similar to ethyl alcohol for equal blood levels but acetone has greater anesthetic potency. It has a low order of oral toxicity but is irritating to the mucous membranes; prolonged dermal contact causes defatting of the skin, which may lead to dermatitis. Acetone is shown to potentiate the hepatotoxicity of chloroform, 1,1,2-TCA, and 1,1,1-TCA as evidenced by increased serum glutamic pyruvic transaminase activity.

Irritation Data:
insufficient information

Oral LD50:
1738 mg/kg (rat)
3000 " (mouse)
9750 " (rat) (10)

Dermal LD50:
20,000 mg/kg (rabbit) (10)
>7,400 " ( " )

Aquatic LC50 (96 hrs):
>1000 ppm

Mutagenicity:
Cytogenic Effect - 200 mmol/tube (*Saccharomyces cerevisiae*)

Carcinogenicty:
Insufficient information. Tumorigenic in hamsters (3).

Reproductive Effects:
insufficient information

Teratogenic Effects:
Teratogenic in insects and chick embryos (3).

## III. STANDARDS

insufficient information

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 10 |
| Bioaccumulation | 0 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0 |
| aquatic LC50: | 0 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 3 |

# BENZENE

File Name: B:Benzene
NIOSH# CY1400000

## I. CHEMICAL INFORMATION

Synonyms:
- Benzol
- Cyclohexatriene
- Annulene
- Coal Naptha
- Phene
- Phenyl Hydride
- Pyrobenzol

Structure:

Physical Properties (11 except where noted):
Mol. Wt.: 78.12
Melting Pt.: 5.5 C
Boiling Pt.: 80.1 C
Vapor Pressure: 95.2 torr (25 C)
Solubility: 1750 mg/l (10 C)
1800 mg/l (25 C)
Kow: 1.95-2.13
Ksc: ~1.95-2.13

Uses (2):

Benzene is produced as a byproduct of the petroleum and coke oven industries. It has widespread use in the chemical and drug industries and as a solvent for paints, resins, lacquers, and plastics. It is a constituent of motor fuels and large quantities are utilized as a starting material in the synthesis of a variety of aromatic products.

Detection (11):

Benzene has been detected in finished drinking water, in water and sediment samples, and in the atmosphere.

Fate in the Environment (11):

Volatilization: Volatilization is the primary transport process.

Photolysis: Photolysis is not significant.

Sorption: Sorption may be significant under constant exposure.

Oxidation: Catalysts, high temperatures, high pressures, or a combination of the above may serve as initiators of benzene oxidation (no info on oxidation under ambient conditions).

Hydrolysis: Probably not a significant fate process.

Bioaccumulation: Kow shows a low bioaccumulation potential.

Biotransformation/Biodegradation: Since benzene is relatively soluble in water, some benzene is expected to persist in the water column. That portion of benzene which persists in the water column would be expected to eventually biodegrade at a slow rate. The biodegradation of benzene would probably be enhanced by the prescence of other hydrocarbons. Some species of soil bacteria have been demonstrated to be capable of utilizing benzene as the sole source of carbon.

## II. TOXICITY INFORMATION

Benzene can act as an accumulative poison. Acute poisoning is accompanied by dizziness, drunkenness, unconsciousness, and finally death. Acute dermal exposure will cause erythemia, scaling, burning, and cracking of the skin, with edema and blistering in severe cases. A full list of symptoms of exposure are as follows: anemia, anorexia, CNS depression, coma, convulsions, dizziness, epistaxis, euphoria, headache, menstrual disturbance, mental confusion, mydriasis, nausea and vomiting, pulmonary edema, purpura, rapid respiration, speech problems, tightness in chest, tremors, urine color change, visual blurring, weakness, and weight loss. (3) Reported in EPA TSCA inventory, 1980. (10)

Irritation Data:
insufficient information

Oral LD50 (10):
3800 mg/kg (rat)
4894 " ( " )
4700 " (mouse)

Oral LD (low) - 130 mg/kg (humans)

Dermal LD (low):
1200 gm/kg (mouse) (10)

Aquatic LC50 (96 hrs):
100-10 ppm (10)

Mutagenicity (10):

| | |
|---|---|
| dlt-rat-orl | 1 mg/kg |
| cyt-hmn:leu | 1 mmol/l/72 hrs |
| cyt-hmn:leu | 1 ppm |
| cyt-smc | 12 mmol/l |
| oms-nml-ipr | 75 gm/kg |
| dni-hmn-ihl | 125 ppm/1 Y |
| cyt-hum-unk | 10 ppm/4 W |
| sce-hmn:lym | 200 umol/l |
| dni-rat-ihl | 400 ppm |
| oms-rat-scu | 1 gm/l |
| cyt-rat-ihl | 300 mg/m3/16 W |
| cyt-rat-scu | 440 mg/kg |

15 other studies noted (mnt, otr, dni, sce, dlt, otr tests)

Reported in EPA Genetic Toxicology Program, 1/84.

Carcinogenicity:

Animal experiments have not clearly demonstrated that Benzene is a carcinogen, but an international ad hoc working group of experts in cancer research concluded from epidemiological data in January 1979 that Benzen is "carcinogenic for humans". (3) Reported in the NTP 3rd Annual Report on Carcinogens, 1982. (10)

Reproductive Effects:

| | | | |
|---|---|---|---|
| orl-mus | TDlo: | 9 gm/kg | (6-15D preg) |
| orl-mus | " | 12 " | ( " " ) |

Also 5 inhalation studies noted.

Teratogenic Effects:

Benzene is a confirmed teratogen (12,13). Female rats and mice exposed to up to 209.7 ppm benzene in the air or to subcutaneous injections of benzene showed sterility, resorption of embryos, and/or skeletal deformities in their offspring. In one study, however, no increase in fetal resorptions was seen when exposure was to 100-2000 ppm. (3)

## III. STANDARDS (5 except where noted)

EPA adjusted acceptable daily intake (ADI): 0.025 mg/l

Proposed upper limit lifetime cancer risks 1/100,000:

| CAG | proposed CAG | NAS |
|---|---|---|
| 6.7 | - | - |

DOHS recommended action level: 0.7 ppb (17)

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 6 |
| Bioaccumulation | 2 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 3 |
| Carcinogenicity | 10c |
| Mutagenicity | 10 |

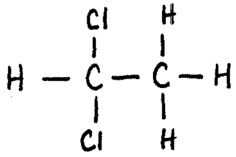
# 1,1-DICHLOROETHANE

File Name: B:1,1-DCA
NIOSH# KI0175000

## I. CHEMICAL INFORMATION

Synonyms:
- Ethylidene Chloride
- Ethylidene Dichloride
- Chlorinated Hydrochloric Ether

Structure:



$\mathrm{H-\underset{Cl}{\overset{Cl}{C}}-\underset{H}{\overset{H}{C}}-H}$

Physical Properties (11)
Mol. Wt.: 98.96
Melting Pt.: -96.98 C
Boiling Pt.: 57.28 C
Vapor Pressure: 180 torr (20 C)
Solubility: 5,500 mg/l (20 C)
Kow: 1.79
Ksc: ~1.9

Uses (12):

1,1-DCA is a flammable liquid with limited use as a solvent and as a chemical intermediate. Formerly used as an anesthetic, it is of no importance in the field today.

Detection (11):

1,1-DCA has been detected in finished drinking water by the National Organics Reconnaissance Survey (NORS). It is present in ambient and upland waters due to absorption of chloroorganics from the atmosphere by water and return to the earth during precipitation.

Fate in the Environment (11 except where noted):

Volatilization: Volatilization should be primary transport process based on high vapor pressure.

No specific information on photodissociation, oxidation, or hydrolysis in water.

Bioaccumulation: 1,1-DCA does not bioaccumulate to any significant extent (11). Chlorinated ethanes exhibit greater bioconcentrating potential with increased chlorination (3).

Biotransformation/Biodegradation: 1,1-DCA included in list of synthetic organic chemicals which should be degradable by biological sewage treatment provided suitable acclimitization can be achieved. Some evidence that 1,2-DCA can be metabolized by fish and oysters - 1,1-DCA may be metabolized as well.(11) One study reported little microbial degradation of chlorinated ethanes in water but did report chemical degradation (3).

## II. TOXICITY INFORMATION (10 except where noted)

Liver injury has been reported in experimental animals following acute exposures ranging from 4,000 to 17,500 ppm (4). Exposure can cause CNS damage. Highly toxic fumes of phosgene are emitted when 1,1-DCA is heated to decomposition. (3)

Oral LD50:
725 mg/kg (rat)

Dermal LD50:
insufficient information

Aquatic LC50:
insufficient information

Mutagenicity:
Not mutagenic in ames test (3).

Carcinogenicity:
NCI bioassay results: indefinite (mouse, rat) (3). Tumorigenic in mice (10).

Teratogenic Effects:
Teratogenic in animal models. (12)

Reproductive Effects:
1 reference of reproductive effect in rats (route inhalation) - lowest dose effect 6,000 ppm/7 hrs.

## III. STANDARDS

no information found

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 7 |
| Bioaccumulation | 1 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 0-10 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 0 |

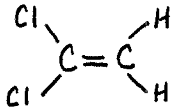
## 1,1-DICHLOROETHENE

File Name: B:1,1-DCE
NIOSH# YZ8061000

### I. CHEMICAL INFORMATION

Synonyms (11):
Vinylidine Chloride
1,1-Dichloroethylene

Structure:



Physical Properties (11 except where noted)

| | | | |
|---|---|---|---|
| Mol. Wt.: | 96.94 | Solubility: | 400 (11) - 2,500 (4) mg/l (20 C) |
| Melting Pt.: | -122.1 C | Kow: | 0.73 (4) - 1.48 (11) |
| Boiling Pt.: | 37 C | | |
| Vapor Pressure: | 591 torr (25 C) | | |

Uses (4)

DCE's are clear colorless liquids. 1,1-DCE is used as a chemical intermediate in the synthesis of methylchloroform and in the production of polyvinylidene chloride copolymers (PVDC). Among other monomers used with 1,1-DCE in copolymer production are vinyl chloride, acrylonitrile, and alkyl acrylates. Polymers with a high PVDC content are widely used in the food packaging industry (e.g. Saran wrap).

Detection (11):

1,1-DCE has been detected in finished drinking water by the National Organics Reconnaissance Survey (NORS). It is also present in ambient and upland waters due to absorption of chloroorganics from the atmosphere by water and return to the earth during precipitation.

Fate in the Environment (11 except where noted):

Volatilization: 1,1-DCE is short-lived in the environment due to volatilization. (4) It appears to be the primary transport process.

Photolysis: Photolysis in aqueous systems is negligible (11). 1.1-DCE's unsaturated bond is subject to photochemical attack (3).

Oxidation: No information found for aquatic systems.

Sorption: No information of sorption found.

Hydrolysis: Probably occurs too slowly to be a significant fate process.

Bioaccumulation: 1,1-DCE is not considered a significant bioaccumulator due to its low Kow.

Biotransformation/Biodegradation: Most studies indicate that low molecular weight chloroaliphatics are not metabolized by microorganisms.

1,1-DCE will sink in water and remain on the bottom; it may smother benthic life.

## II. TOXICITY INFORMATION (10 except where noted)

There is a correlation between the degree of water chlorination and the toxicity of DCE. DCE's are anesthetics. They are metabolically converted to reactive epoxide intermediates. (4) In direct contact 1,1-DCE is a mild irritant (3). Non-carcinogenic effects (at high doses) include liver and kidney damage, renal toxicity, CNS depression and sensitization of the heart (5).

Irritation Data:
insufficient information

Oral LD50:
200 mg/kg (rat)

Dermal LD (low):
4840 mg/kg (mouse)

Aquatic LC50 (96 hrs):
1000-100 ppm

Mutagenicity:

| | |
|---|---|
| mma-sat | 2 pph/4 H |
| mma-smc | 20 mmol/L |
| mrc-smc | 20 mmol/L |
| hma-mus/smc | 400 mg/kg |

Carcinogenicity:
IARC determination: Animal positive (3).

Reproductive Effects:
1 ref. of reproductive effect (oral route) - study on rats - lowest dose effect at 1 gm/kg (14 wks on males before mating, 14 wks on females before mating, 3 wks post-partum).

Teratogenic Effects:
Teratogenic in rabbits (4).

## III. STANDARDS

EPA water quality criteria to protect human health (4):

| | Increased Cancer Risk (ug/l) | | |
|---|---|---|---|
| 1/ | 100,000 | 1,000,000 | 10,000,000 |
| Ambient Water Concentration | 0.33 | 0.033 | 0.003 |
| Consumption of Aquatic Organisms Only | 18.5 | 1.85 | 0.185 |

EPA Acute Toxicity Limits (4):
Freshwater: 11,600 ug/l
Saltwater: 224,000 ug/l

EPA adjusted acceptable daily intake (ADI): 0.35 mg/l (5)

Projected upper limit lifetime cancer risks 1/100,000 (5)

| CAG | proposed CAG | NAS | |
|---|---|---|---|
| 2.3 | 2.4 | - | ug/l |

DOHS recommended action level: limit of detection (0.10-0.4 ppb) (17)

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 8-10 |
| Bioaccumulation | 0 |
| Acute Toxicity | |
| oral LD50: | 3 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 1 |
| Carcinogenicity | 10b |
| Mutagenicity | 3-10 |

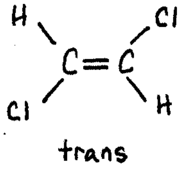
# 1,2-DICHLOROETHENE
## (cis- and trans- isomers)

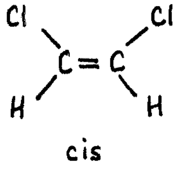
File Name: B:1,2-DCE
NIOSH# KV9360000

## I. CHEMICAL INFORMATION

Synonyms (11):
- trans-1,2-Dichloroethylene
- trans-Acetylene Dichloride
- Dioform
- cis-1,2-Dichloroethylene
- cis-1,2-Acetylene Dichloride

Structure:


trans


cis

Physical Properties (11 except where noted):
Mol. Wt.: 96.94
Melting Pt.: -50 C
Boiling Pt.: 47.5 C
Vapor Pressure: 324 torr (4)
Solubility: 600 (11) - 6,300 (4) mg/l (20 C)
Kow: 1.48
Ksc: ~1.5

1,2-Dichloroethylene always consists of a mixture of the cis and trans isomers with the relative proportions of the isomers depending upon production conditions. (3) 1,2-DCE is relatively stable when compared to 1,1-DCE due to symetric chlorine substitution (6). Both isomers dimerize to tetrachlorobutane in the prescence of organic peroxides. Contact of the solvent with sodium or sodium caustic alkalies, copper or copper alloys may release chlroacetylene, which is explosive, spontaneously flammable in air, and toxic. (3)

Uses (3):

1,2-DCE is used as a general solvent for organic materials (fats, phenol, camphor); for extraction of dyes, caffeine, perfumes; for lacquers, thermoplastics, organic synthesis, and for retarding fermentation. It is often produced as a by-product in chlorination reactions and is recycled as an intermediate for the synthesis of more useful chlorinated ethylenes.

Detection (11):

Detected in finished drinking water by the National Organics Reconnaissance Survey (NORS). Present in ambient and upland waters due to absorption of chloroorganics from the atmosphere by water and return to the earth during precipitation.

Fate in the Environment (11 except where noted):
- Volatilization: Volatilization appears to be the primary transport process.
- Photolysis: Photolysis is not significant.
- Sorption: Insufficient information; probably insignificant.
- Oxidation: Photooxidation of 1,2-DCE is more rapid than for PCE & TCE under certain conditions; photooxidative products formic acid, hydrochloric acid, and carbon monoxide.

Hydrolysis: Probably occurs too slowly to be a significant fate process.

Bioaccumulation: Low potential for bioaccumulation due to low Kow.

Biotransformation/Biodegradation: Biodegradation very slow (low molecular weight chloroaliphatics generally not metabolized by microorganisms).

## II. TOXICITY INFORMATION (10 except where noted)

Direct contact may burn the skin and eyes and irritate the respiratory system. CNS depression, conjunctivitis, dizziness, narcosis, nausea, vomiting, weakness, tremor, and cramps can follow 1,2-DCE exposure. Chronic exposures have caused liver and kidney damage in experimental animals. The trans isomer is twice as toxic and anesthetic as the cis isomer. (3) DCE's are metabolically converted to reactive epoxide intermediates (4).

Irritation Data:
insufficient information

Oral LD50:
770 mg/kg (rat)

Dermal LD50:
insufficient information

Aquatic LC50 (96 hrs):
1000-100 ppm

Mutagenicity:

Cis and trans isomers were nonmutagenic when assayed with _E. coli_ K12 and mutagenic with _Salmonella_ tester strains. Dominant lethal tests on adult CD male rats showed negative results. (3,4) The cis isomer promoted chromosomal aberrations in cytogenic analysis of bone marrow cells after repeated intraperitoneal injections in intact animals. The trans isomer did not. (3)

Carcinogenicity:
insufficient information

Teratogenicity:
insufficient information

Reproductive Effects:
insufficient information

## III. STANDARDS (4)

EPA acute toxicity limits:
Freshwater - 11,600 ug/l
Saltwater - 224,000 "

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 8 |
| Bioaccumulation | 0 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 1 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 0-10 |

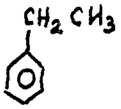
# ETHYL BENZENE

File Name: B:EBEN
NIOSH# DA0700000

## I. CHEMICAL INFORMATION

Synonyms (11):
Phenylethane
Ethylbenzol

Structure:



Physical Properties (11 except where noted):
Mol. Wt.: 106.16
Melting Pt.: -94.9 C
Boiling Pt.: 136.2 C
Vapor Pressure: 7 torr (20 C)
Solubility: 152 mg/l (20 C)
Kow: 3.15
Ksc: ~3.15

Uses (12):

Ethylbenzene is a colorless, flammable liquid with a pungent odor. It is prepared by dehydrogenation of napthenes or from catalytic cyclization and aromatization, but mainly by akylation of benzene. It is used in the production of styrene and synthetic polymers, as a solvent, and as a component for automotive and aviation fuels.

Detection (11):

Detected in finished drinking water, effluents, and ambient surface waters.

Fate in the Environment (11 except where noted):

Volatilization: Volatilization is main transport process in water. Computed Henry constant (H = 6.44 atm. m3 mole-1) is in the same range as Toluene (H = 6.68 atm. m3 mole-1). Therefore, half-life in water assumed to be approx. the same (5-6 hrs. in water layer 1 meter thick).

Photolysis: Photodegradation occurs with this chemical - half life of 35 daylight hours.

Sorption: insufficient information

Oxidation: Ethylbenzene readily oxidized in the liquid phase by molecular oxygen, but this oxidation is effectively inhibited by the prescence of water. No data on rates of oxidation in environmental waters.

Hydrolysis: Probably occurs too slowly to be a significant fate process.

Bioaccumulation: High Kow indicates compound may bioaccumulate in adipose tissue.

Biotransformation/Biodegradation: Some bacteria can use ethylbenzen as sole carbon source. Microbial oxidative degradation proceeds via hydroxylation of the aromatic ring to 2,3-dihydroxy-1-ethylbenzene.

Ethylbenzene will float in a slick in water (3).

## II. TOXICITY INFORMATION (10 except where noted)

Ethylbenzene is an irritant to the skin, eyes, and mucous membranes; it is narcotic in high concentrations. Ethylbenzene has been detected in cord blood samples, indicating its transport through the placenta. Studies on rabbits showed chronic effects on the CNS, growth, morphological composition of blood, and histological changes in organs. (3) Included in EPA TSCA inventory, 1980 (10).

Irritation Data (3,10):
skin rabbit - 15 mg/24 hrs, open - mild
eye rabbit - 100 mg

Oral LD50:
3500 mg/kg (rat) (3,10)

Dermal LD50:
5,000 mg/kg (rabbit) (3)
17,800 mg/kg (rabbit)

Aquatic LC50 (96 hrs):
100-10 ppm

Mutagenicity:
Insufficient information. Included in EPA Genetic Toxicology Program, January 1984.

Carcinogenicity:
Insufficient information. Ethylbenzene selected by NTP for carcinogenesis studies but studies deferred as of 12/83.

Teratogenicity:
Positive results in rat and rabbit studies (3).

Reproductive Effects:
4 Inhalation studies noted (3).

## III. STANDARDS (4)

EPA limits: 32,000 ug/l to protect freshwater organisms
1.4 " " " human health

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 1.5 |
| Bioaccumulation | 4 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 1 |
| aquatic LC50: | 3 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 0-10 |

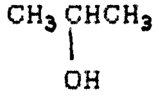
## ISOPROPYL ALCOHOL

File Name: IPA
NIOSH #: NT8050000

## I. CHEMICAL INFORMATION

Synonyms: (10)
- Isopropanol
- 2-propanol
- Dimethyl carbinol
- 1-methylethyl alcohol

Structure: (11)



$CH_3\underset{\displaystyle OH}{\underset{|}{C}}HCH_3$

Physical Properties: (12)

| | | | | |
|---|---|---|---|---|
| Molecular Wt. | | 60.10 | Solubility | infinite |
| Melting Point | | -88.5C | Kow | -0.16 to0.28 |
| Boiling Point | 20C | 82.5C | Ksc | 0 |
| Vapor Pressure | 25C | 44mmHg | Flammable | |

Uses: (12,8)

50% used in manufacture of acetone; also used as solvent in perfumes, oils, gums, resins, extraction processes; used in plastics, dyes, lacquers, liniments, skin lotions, cosmetics, pharmaceuticals, rubbing alcohol, antifreeze, liquid soaps, window cleaners, and mouthwashes.

Detection: (3)

A food additive permitted in food for human consumption; common air contaminant.

Fate in the Environment:

Hydrolysis - will dissolve in freshwater; will float in slick on saltwater (3)

Biodegradation - will biodegrade at moderately fast rate to Acetone (12);
used as sole carbon source in activated sludge (15)

No other information re: environmental processes

## II. TOXICITY INFORMATION

Harmful effects: (14,3)

relatively innocuous; mild irritation of eyes, nose, and throat at 400 ppm;transient narcosis at higher concentrations. Potentiates hepatotoxicity of Carbon tetrachloride; in large amounts, more toxic and narcotic than ethyl alcohol (12).

Irritation Data: (10)

| | | |
|---|---|---|
| eye | human | 20 ppm |
| eye | rabbit | 16 mg |
| skin | rabbit | 500 mg, mild |

Toxicity Data: EPA TSCA, (10)

| | | | |
|---|---|---|---|
| oral | human | TDlo: | 15710 mg/kg |
| oral | man | LDlo: | 8600 mg/kg |
| oral | rat | LD50: | 5840 mg/kg |
| oral | mouse | LDlo: | 192 mg/kg |
| oral | dog | LD50: | 6150 mg/kg |
| oral | rabbit | LDlo: | 5000 mg/kg |
| skin | rabbit | LD50: | 13000 mg/kg |

Aquatic Toxicity: (10)
LC50: 1000-100 ppm

Carcinogenicity:(10)
IARC Determination - human suspected; animal indefinite.
NIOSH suspects carcinogen present in old "strong acid" process for IPA oil; whether carcinogen present in new "weak acid" process not determined (14).

Mutation Data: (10)
EPA Genetic Toxicology Program 1/84.
cytoggenetic analysis -*Saccharomyces cerevisiae*: 200mmol/tube
cytogenetic analysis - rat inhalation: 1030 ug/m /16wk,intermit.

## III. STANDARDS

Permissible Concentration in Water: (14)
No criteria set.
EPA suggested ambient goal for health effects - 13,500ug/L.

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 10 |
| Bioaccumulation | 0 |
| Acute Toxicity | |
| oral LD50: | 0 |
| dermal LD50: | 0 |
| aquatic LC50: | 1 |
| Carcinogenicity | 10a |
| Mutagenicity | 10 |

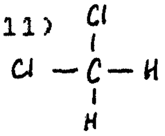
# METHYLENE CHLORIDE

File Name: DCM
NIOSH #: PA8050000

## I. CHEMICAL INFORMATION

Synonyms: (10)
Dichloromethane (DCM)
Methylene bichloride
Methylene dichloride

Structure: (11)
$CH_2Cl_2$



halogenated aliphatic hydrocarbon

Physical Properties: (11,12)

| | | |
|---|---|---|
| Molecular Wt. | | 89.94 |
| Melting Point | | -95.0C |
| Boiling Point | | 39.75C |
| Vapor Pressure | 20C | 362.4 |
| | 25C | 440 |

| | | |
|---|---|---|
| Solubility | 25C | 13.2-20g/L |
| | 20C | 2g/100ml |
| Kow | | 1.25 |
| Ksc | | ~ 1.25 |

Uses: (2)

a volatile solvent with wide general application as an aerosol propellant, paint stripper; degreasing solvent for cellulose esters, fats, oils, resins and rubbers; used in coating photographic films; used as a chemical intermediate in insecticide formulations.

Detection: (11)

Detected in finished drinking water, in the troposphere, and in coffee.

Fate in the Environment: (11)

Volatilization - major transport process for removal from aquatic systems; experimental halflife is 27 minutes.
Photolysis - probably not significant in aquatic systems; estimated halflife is greater than 250 hours.
Oxidation - predominant fate in troposphere; lifetime of 0.30 years.
Hydrolysis - probably not significant; halflife=417 days
Sorption - probably not significant
Bioaccumulation - probably not significant
Biotransformation/Biodegradation - probable, but at extremely slow rate

## II. TOXICITY INFORMATION

Harmful effects: (14)

Local- dermatitis; irritating to eyes and upper respiratory tract at high concentrations.

Systemic- mild narcotic; severe exposure may cause toxic encephalopathy with hallucinations, pulmonary edema, coma, and death; metabolized to CO and may cause increase in carboxyhemoglobin levels which may be significant in smokers or workers with anemia, heart disease; additive effect with CO exposure.

Irritation Data: (10)
skin rabbit 810 mg/24 hours, severe
eye rabbit 162 mg, moderate; 10 mg, mild

Toxicity Data: EPA TSCA, (10)
oral rat LD50: 2136 mg/kg
oral dog LDlo: 3000 mg/kg
oral rabbit LDlo: 1900 mg/kg

Aquatic Toxicity: (10)
LC50: 1000-100 ppm

Carcinogenicity: (10,12)
IARC Determination - animal indefinite
NTP Carcinogenesis Study completed 12/83

Tumorigenic Data - inhalation rat TClo: 500ppm/6hr/2yr Statistically significant dose related response - increase in sarcomas (malignant mesenchymal tumors) at 3500ppm exposure (12).

Mutation Data: (10)
EPA Genetic Toxicology Prgram 1/84
mutation in microorganisms -*Salmonella typhimurium*: 5700 ppm
microsomal mutagenicity assay - *S. typhimurium*: 5700 ppm
sex chromosome loss & nondisjunction - *Drosophila melanogaster* - oral: 125 mmol/L
DNA inhibition - human - fibroblast: 5000 ppm/1hr continuous
oncogenic transformation - rat - embryo: 160 umol/L
oncogenic transformation - hamster - embryo: 1300 uL/plate
DNA inhibition - hamster - lung: 5000 ppm/1hr continuous
sister chromatid exchange - hamster - lung: 5000 ppm/1hr cont

Reproductive Data: (10)
inhalation rat TClo: 4500 ppm/24hr (1-17 days pregnant)
inhalation rat TClo: 1250 ppm/7hr (6-15 days pregnant)
inhalation mouse TClo: 1250 ppm/7hr (6-15 days pregnant)

Teratogenicity:
no teratogenic effect observed (7).
low degree maternal/embryo toxicity; young of exposed pregnant rats showed retarded behavioral habitation to new environment; unable to determine if due to carboxyhemoglobin (12).

## III. STANDARDS

EPA Priority Pollutant
Permissible Concentration in Water: (14)
To protect human health - preferable zero
Additional lifetime cancer risk of 1/100,000
at 1.9 ug/L ambient water
at 157 ug/L ingestion of aquatic organisms only
DOHS Action Level - 40 ppb
EPA criterion level for non-cancer effects - 12.4 ppm (4).

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 9 |
| Bioaccumulation | 0 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0-10 |
| aquatic Lc50: | 1 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 10 |

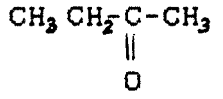
## METHYL ETHYL KETONE

File Name: MEK
NIOSH #: EL6475000

## I. CHEMICAL INFORMATION

Synonyms: (10)
- 2-Butanone
- Butanone
- Methyl acetone

Structure: (12)



$CH_3CH_2\text{-}\overset{\displaystyle O}{\overset{\|}{C}}\text{-}CH_3$

aliphatic ketone

Physical Properties: (12)

| | | | |
|---|---|---|---|
| Molecular Wt. | 72.10 | Flammable liquid | |
| Melting Point | -86C | Solubility | $26g/100gH_2O$ |
| Boiling Point | 80C | Kow | 0.26 |
| Vapor Pressure 20C | 77.5 | Ksc | 0.2 |

Uses: (8)

Ketones are used as solvents for oils, fats, collodion, cellulose acetate, nitro cellulose, cellulose esters, epoxy resins, dyes, vinyl polymers, acrylic coatings;
used in manufacture of paints, lacquers, varnishes, rubber, artificial leather, explosives; in metal cleaning, airplane dopes, and hydraulic fluids.

Detection: no information

Fate in the Environment: no information

## II. TOXICITY INFORMATION

Harmful effects: (14,8)

irritation of eyes and nose; headaches, dizziness, vomiting; at high concentrations, central nervous system depression and narcosis may occur.
Potentiating effect of MEK indicated in mixed exposure with Methyl Butyl Ketone.

Irritation Data: (10)

| | | |
|---|---|---|
| eye | human | 350 ppm |
| skin | rabbit | 500 mg/24hr, moderate; 402 mg/24hr, mild |
| skin | rabbit | 13780 ug/24hr open, mild |
| eye | rabbit | 80 mg |

Toxicity Data: EPA TSCA, (10)

| | | |
|---|---|---|
| oral | rat | LD50: 2737 mg/kg |
| dermal | rabbit | LD50: 13000 mg/kg |

Aquatic Toxicity: (10)
LC50: >1000 ppm

Carcinogenicity: no information

Mutagenicity:
EPA Genetic Toxicology Program 1/84

Reproductive Effects Data: (10)
inhalation rat TClo: 1000 and 3000 ppm/7hr 6-15days preg.

## III. STANDARDS

Not on EPA Priority Pollutant List
Permissible Concentration in Water:(14)
No criteria set

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 10 |
| Bioaccumulation | 0 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0 |
| aquatic LD50: | 0 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 0-10 |

# PHENOL

File Name: Phenol
NIOSH #: SJ3325000

## I. CHEMICAL INFORMATION

Synonyms: (10)
Carbolic acid
Phenyl alcohol
Baker's P&S liquid & ointment

Structure: (11)
$C_6H_5OH$

Physical Properties: (11)

| | | | |
|---|---|---|---|
| Molecular Wt. | 94.11 | Solubility 25C | 93000mg/L |
| Melting Point | 40.90C | Kow | 1.46 |
| Boiling Point | 181.75C | Ksc | 1.5 |
| Vapor Pressure 20C | 0.5293torr | | |

Uses: (12)
Used in production/manufacturing of aromatic compounds including explosives; in fertilizers, coke, illuminating gas, lampblack, paints, paint removers, rubber, asbestos goods, wood preservatives, resins, textiles, drugs, perfumes, bakelite, other plastics; in petroleum, leather, paper, soap, toy, and agricultural industries.

Detection: (11)
Detected in finished drinking water, surface water, and industrial effluents.

Fate in the Environment: (11)
Volatilization - possible but low VP and high solubility imply little tendency; highly solvated/persistent in water
Photolysis - in aerated surface water
Hydrolysis - not relevant
Oxidation - metal catalyzed in some aerated surface water
Sorption - not significant; very little affinity for microcrystalline clay particulates; ineffective as flocculant of clays and soils
Bioaccumulation - not significant
Biotransformation/Biodegradation - a very significant fate process in aqueous media with sufficient concentration of microorganisms; primary carbon source for mixed population of soil organisms; Goldfish also able to biotransform.
*Additive effect for combinations of different phenols; toxicity increases with salinity (3).
Other Reactions - chlorophenols may be produced in advertently by chlorination process for drinking water sources.

## II. TOXICITY INFORMATION

Harmful effects: (14)
Local - marked corrosive effect on any tissue; eye contact may cause severe damage and blindness; skin contact causes

whitening of area or burns.

Systemic - from any route of exposure; paleness, weakness, sweating, headache, tinnitis, shock, cyanosis, excitement, frothing of the nose and mouth, dark colored urine, death. If death does not occur, kidney damage may occur; chronic hazard includes renal and hepatic damage.

Irritation Data: (10)

| | | | |
|---|---|---|---|
| skin | rabbit | 500 mg/24 hr | severe |
| skin | rabbit | 535 mg open | severe |
| eye | rabbit | 5 mg | severe |

Toxicity Data: EPA TSCA, (10)

| | | | |
|---|---|---|---|
| oral | human | LDlo: | 140 mg/kg |
| oral | rat | LD50: | 414 mg/kg |
| skin | rat | LD50: | 669 mg/kg |
| oral | rabbit | LDlo: | 420 mg/kg |
| skin | rabbit | LD50: | 850 mg/kg |
| oral | mouse | LD50: | 282 mg/kg |
| oral | dog | LDlo: | 500 mg/kg |
| oral | cat | LDlo: | 80 mg/kg |

Aquatic Toxicity: (10)

LC50: 100-10 ppm

Carcinogenicity: (10)

NCI Carcinogenesis bioassay completed;

Results - Negative mouse, rat

Tumorigenic Data: (10)

| | | | |
|---|---|---|---|
| skin | mouse | TDlo: | 16 gm/kg/40 wk intermittent |
| skin | mouse | TD: | 4 gm/kg/24 wk intermit |

Mutagenicity: (10)

EPA Genetic Toxicology Program 1/84

| | |
|---|---|
| mutation in microorganism - *Salmonella typhimurium*: | 400 uL/plate |
| microsomal mutagenicity assay - *S. typhimurium*: | 40 umol/plate |
| sex chromosome loss & nondisjunction - *Drosphila melanogaster*, ovary: | 100 ppm |
| DNA inhibition - human fibroblast: | 10 mmol/L |
| DNA inhibition - human HeLa cell: | 1 mmol/L |
| sister chromatid exchange - human lymphocyte: | 200 umol/L |
| DNA inhibition - mouse oral: | 20 gm/kg |
| DNA damage - mammalian lymphocyte: | 250 mmol/L |

Reproductive Effects Data: (10)

intraperitoneal rat TDlo: 600 mg/kg 12-14 days pregnant

## III. STANDARDS

EPA Priority Pollutant

Permissible Concentration in Water: (14,4)

To protect freshwater aquatic life - acute = 10,200 ug/L
chronic = 2,560 ug/L

To protect saltwater aquatic life - acute = 5,800 ug/L

To protect human health from contaminated water and aquatic organism ingestion - 3.5 mg/L
To protect against organoleptic effects - 0.3 mg/L

DOHS Action Level for chlorinated systems organoleptic effects - 1 ppb

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 8 |
| Bioaccumulation | 0 |
| Acute Toxicity | |
| oral LD50: | 3 |
| dermal LD50: | 1 |
| aquatic LD50: | 3 |
| Carcinogenicity | 0 |
| Mutagenicity | 10 |

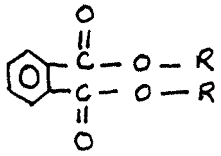
# PHTHALATE ESTERS

File Name: P.Esters

| | | | |
|---|---|---|---|
| NIOSH #: | Dimethyl phthalate | TI1575000 | DMP |
| | Diethyl phthalate | TI1050000 | DEP |
| | Di-n-butyl phthalate | TI0875000 | DBP |
| | Di-n-octyl phthalate | TI1925000 | DOP |
| | Bis(2-ethylhexyl) phthalate | TI0350000 | DEHP |
| | Butyl benzyl phthalate | TH9990000 | BBP |

## I. CHEMICAL INFORMATION

Synonyms and Structures: (11)
See Attachment #1



Physical Properties: (11)
See Attachment #2

Uses: (2,12)

Phthalate esters are among the most important industrial chemicals, used in virtually every major product category including construction, automotive, household products, apparel, toys, packaging, and medical products (dentistry and surgery as plastic components, vinyl plastic bags for blood storage); used as food packaging component.

With liquid carrier, methyl and ethyl phthalates serve as effective insect repellants.

Most abundantly produced esters are DEHP and DBP.

Detection: (11,2)

Ubiquitously distributed in environment; general contaminants of virtually all soil and water ecosystems; complexed with fulvic acid components of humic substances in soil, and marine and estuarine waters; detected in open ocean, drinking water, well water, oil, air, plants, fish, food, animals, humans. May be biosynthesized.

Fate in the Environment: (11)

Insufficient data to predict predominant process.

Volatilization - not significant, with possible exception of those esters with low solubility, i.e., DEHP, BBP

Photolysis - not relevant

Oxidation - not significant

Hydrolysis - very slowly, not significant; specific aquatic halflives calculated:

DMP = 3.2yrs DEHP = 2000yrs DEP = $\sim$18.3yrs DBP = $\sim$10yrs

Sorption - probably principal aquatic transport mechanism; onto suspended particulates and biota, and complexation with humic substances; transport dependent on hydrogeologic conditions.

Bioaccumulation - an important fate process; a variety of organisms take up and accumulate phthalate esters, especially DEHP, DBP, DOP;
lipophilic but not likely to biomagnify; aquatic organisms more apt to concentrate P. esters than warm blooded animals.

Biotransformation/Biodegradation - an important fate process; several microorganisms able to utilize selected P.esters as sole carbon and energy source;
degraded under most conditions and metabolized by multicellular organisms, especially for DEHP, DBP, DOP;
halflife for DEHP is ~4 weeks reported in laboratory study of river water.

## II. TOXICITY INFORMATION

### A. Dimethyl phthalate

Harmful effects: (14)
irritation of nasal passages and upper respiratory system; stomach irritation; eye pain.

Irritation Data: (10)
eye rabbit 119 mg

Toxicity Data: (10)
oral rat LD50: 6900 mg/kg
oral mouse LD50: 7200 mg/kg
oral rabbit LD50: 4400 mg/kg
oral guinea pig LD50: 2400 mg/kg

Aquatic Toxicity: (11)
LC50: 33 ppm fresh water; 58 ppm saltwater

Carcinogenicity: (10)
NTP Carcinogenesis Study 1983; status not given

Mutation Data: (10)
mutation in microorganism - Salmonella typhimurium: 5 mmol/L
cytogenetic analysis - rat skin: 25 gm/kg/4wk intermittent

Reproductive Effects Data: (10)
intraperitoneal rat TDlo: 338 and 1125 mg/kg 5-15d preg

### B. Diethyl phthalate

Harmful effects: (14)
little effect on skin; vapor exposure causes irritation to nose and throat, conjunctivitis, corneal necrosis, respiratory tract irritation, dizziness, nausea, and eczema.

Irritation Data: (10)
eye rabbit 112 mg

Toxicity Data: (10)
oral rat LD50: 9000 mg/kg
oral mouse LD50: 6172 mg/kg
oral rabbit LDlo: 1000 mg/kg

Aquatic Toxicity: (11)
LC50: 7.59 ppm saltwater; 52.1 ppm freshwater

Carcinogenicity: (10)
selected for NTP Carcinogenesis study 12/83

Mutagenicity: (10)
mutation in microorganisms - *Salmonella typhimurium*: 1100 mmol/L

Reproductive Effects Data: (10)
intraperitoneal rat TDlo: 506 mg/kg 5-15d preg

Teratogenic and fetal toxicity effects reported (14)

## C. Di-n-butyl phthalate

Harmful effects:
irritation of nasal passages and upper respiratory system;
stomach irritation; light sensitivity.

Toxicity Data: (10)
oral human TDlo: 140 mg/kg
oral rat LD50: 8000 mg/kg
oral mouse LD50: 5282 ug/kg

Aquatic Toxicity: (11)
LC50: .730 ppm freshwater

Mutation Data: (10)
EPA Genetic Toxicology Program 1/84
mutation in microorganism - *Salmonella typhimurium*: 90 umol/L
cytogenetic analysis - hamster fibroblast: 30 mg/L/24 hr

Reproductive Effects Data: (10)
oral rat TDlo: 8400 ug/kg 7days male
oral rat TDlo: 2520 mg/kg 1-21days preg
oral rat TDlo: 12600 mg/kg 1-21days preg
intraperitoneal rat TDlo: 1017 mg/kg 5-15days preg
intraperitoneal rat TDlo: 305 mg/kg 5-15days preg
intraperitoneal rat TDlo: 6000 mg/kg 3-9days preg
oral mouse TDlo: 21600; 8640; 1080 mg/kg 1-18d preg
oral mouse TDlo: 16800 mg/kg 7day male
oral guinea pig TDlo: 14000 mg/kg 7day male

## D. Di-n-octyl phthalate

Harmful effects: no information re: acute toxicity symptoms

Irritation Data: (10)
skin rabbit 500 mg/24 hr mild
eye rabbit 5 mg severe

Toxicity Data: (10)
oral mouse LD50: 6513 mg/kg

Aquatic Toxicity: no information

Reproductive Effects Data: (10)
intraperitoneal rat TDlo: 5000 mg/kg 5-15days preg

Teratogenic and fetal toxicity reported (14)

E. Butyl benzyl phthalate
Harmful effects: no information

Toxicity Data: (10)
oral rat LD50: 2330 mg/kg
oral mouse LD50: 4170 mg/kg

Aquatic Toxicity: (11)
LC50: 1.7 ppm freshwater; .9 ppm saltwater

Carcinogenicity: (10)
NTP Carcinogenesis bioassay completed 12/83;
Results - indefinite rat; negative mouse
IARC Determination - animal indefinite
Reselected by NTP for Carcinogenesis studies 12/83

Tumorigenic Data:
oral rat TDlo: 433 gm/kg/2 yr continuous

F. Bis(2-ethylhexyl) phthalate
Harmful effects: (14)
irritation of eyes and mucous membranes; nausea, diarrhea.

Irritation Data: (10)
skin rabbit 500 mg/24 hr mild
eye rabbit 500 mg/24 hr mild

Toxicity Data: (10)
oral man TDlo: 143 mg/kg
oral rat LD50: 31000 mg/kg
oral mouse LD50: 30000 mg/kg
oral rabbit LD50: 34000 mg/kg
skin rabbit LD50: 25000 mg/kg
oral guinea pig LD50: 26000 mg/kg
skin guinea pig LD50: 10000mg/kg

Aquatic Toxicity: (11)
LC50: 11.1 ppm freshwater

Carcinogenicity: (10)
NTP Carcinogenesis bioassay completed:
Results - Positive mouse, rat
IARC Determination - animal Positive, human indefinite

Tumorigenic Data:
oral rat TDlo: 216 gm/kg/2 yr continuous
oral rat TD: 433 gm/kg/2 yr cont
oral mouse TDlo: 260 gm/kg/2 yr cont
oral mouse TD: 519 gm/kg/2 yr cont

Mutation Data: (10)
EPA Genetic Toxicology Program 1/84
microsomal mutagenicity assay - *Salmonella typhimurium*: 5mg/plate
cytogenetic analysis - human leukocyte: 6 mg/L
dominant lethal test - mouse intraperitoneal: 12780 mg/kg
dominant lethal test - mouse subcutaneous: 3 gm/kg/10d intermit
oncogenic transformation - hamster oral: 750 mg/kg
cytogenetic analysis - hamster oral: 7500 mg/kg

Reproductive Effects Data: (10)
oral rat TDlo: 7140 mg/kg 1-21d preg
oral rat TDlo: 35 mg/kg 14d male/14d pre
oral rat TDlo: 8400 ug/kg 7d male
oral rat TDlo: 17200 mg/kg (MGN)
oral rat TDlo: 43000 mg/kg (MGN)
oral mouse TDlo: 16800 mg/kg 7d male
oral mouse TDlo: 50 mg/kg 7d preg
oral mouse TDlo: 1000 mg/kg 7d preg
oral mouse TDlo: 3420 mg/kg 1-18d preg
oral mouse TDlo: 2040 mg/kg 1-17d preg
oral guinea pig TDlo: 20000 mg/kg 10d male
oral mammalian TDlo: 20000 mg/kg 10d male
Data also by intraperitoneal, subcutaneous, intravenous routes.

## III. STANDARDS

All 6 esters EPA Priority Pollutants
Permissible Concentrations in Water: (14)
To protect freshwater aquatic life - acute = 940 ug/L
chronic = 3 ug/L
To protect saltwater aquatic life - chronic = 2944 ug/L

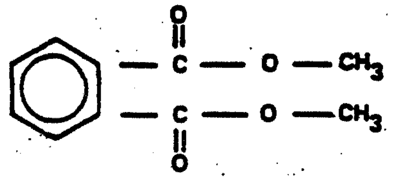
EPA ambient water criterion to protect human health (4):
DMP = 313 mg/L
DEP = 350 mg/L
DBP = 34 mg/L
DEHP = 15 mg/L
no information for DOP, BBP

EPA ambient water criterion for ingestion of contaminated aquatic organisms alone (4):
DMP = 2.9 g/L
DEP = 1.8 g/L
DBP = 154 mg/L
DEHP = 50 mg/L

## IV. RANKING

| | | |
|---|---|---|
| Soil Sorption | 0-5.5 | |
| Bioaccumulation | 2-10 | |
| Acute Toxicity | | |
| oral LD50: | 1 | BBP, DMP |
| dermal LD50: | 0 | DEHP |
| aquatic LC50: | 10 | DBP |
| Carcinogenicity | 10b | DEHP |
| Mutagenicity | 10 | DMP, DEP, DBP, DEHP |

Attachment #1



Dimethyl phthalate

CAS NO. 131-11-3
TSL NO. TI 15750

**Alternate Names**

DMP
1,2-Benzenedicarboxylic acid, dimethyl ester
Phthalic acid dimethyl ester
Methyl phthalate

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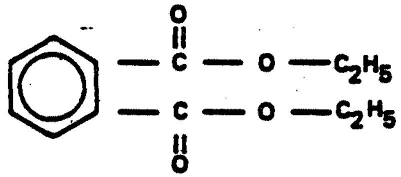


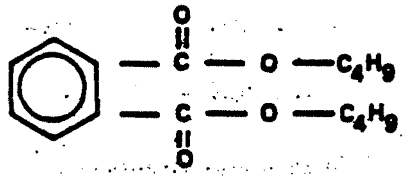
Diethyl phthalate

CAS NO. 84-66-2
TSL NO. TI 10500

**Alternate Names**

DEP
1,2-Benzenedicarboxylic acid, diethyl ester
Ethyl phthalate

---



Di-n-butyl phthalate

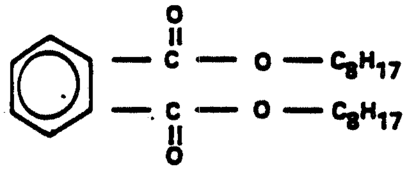
CAS NO. 84-74-2
TSL NO. TI 08750

**Alternate Names**

DBP
o-Benzenedicarboxylic acid, dibutyl ester
Dibutyl phthalate
Benzene-o-dicarboxylic acid, di-n-butyl ester
n-Butyl phthalate

94-2

Attachment #1



Di-n-octyl phthalate

CAS NO. 117-84-0
TSL NO. TI 19250

**Alternate Names**

DOP
o-Benzenedicarboxylic acid, dioctyl ester
n-Dioctyl phthalate
Octyl phthalate
Dioctyl-o-benzenedicarboxylate

---

*Di-n-octyl phthalate is sometimes mistakenly reported as its isomer, bis(2-ethylhexyl) phthalate, in the literature.

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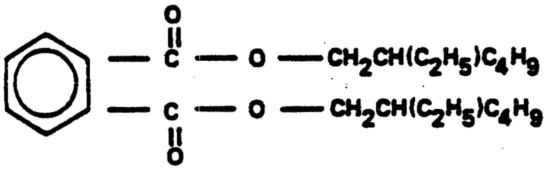


Bis (2-ethylhexyl) phthalate

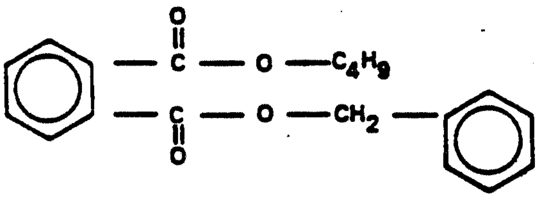
CAS NO. 117-81-7
TSL NO. TI 03500

**Alternate Names**

DEHP
Di(2-ethylhexyl) phthalate
Bis(2-ethylhexyl) ester, phthalic acid
Di-sec-octyl phthalate
Di(2-ethylhexyl) orthophthalate
2-Ethylhexyl phthalate
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester

---

*Bis(2-ethylhexyl) phthalate is sometimes mistakenly reported as its isomer, di-n-octyl phthalate (DOP), in the literature.



Butyl benzyl phthalate

CAS NO. 85-68-7
TSL NO. TH 99900

**Alternate Names**

BBP
Benzyl butyl phthalate

## Table 94-1

## Physical Properties of Phthalate Esters

| | dimethyl | diethyl | di-n-butyl | di-n-octyl | bis(2-ethylhexyl) | butyl benzyl |
|---|---|---|---|---|---|---|
| Molecular weight | 194.18[a] | 222.23[a] | 278.34[b] | 391.0[a] | 391.0[a] | 312.0[c] |
| Melting point | 0°C[d] | -40.5°C[a] | -35°C[d] | -25°C[a] | -50°C[a] | -35°C[e] |
| Boiling point | 282°C(760 torr)[d] | 298°C(760 torr)[d] | 340°C(760 torr)[a] | 220°C(4 torr)[a] | 386.9°C(5 torr)[a] | 377°C(760 torr)[e] |
| Vapor pressure | <0.01 torr(20°C)[a] | 0.05 torr(70°C)[a] | 0.1 torr(115°C)[a] | <0.2 torr(150°C)[a] | <0.01 torr(20°C)[a]<br>$2 \times 10^{-7}$ torr (20°C)[f] | Not available |
| Solubility | 5000 mg/l(20°C)[c]<br>4000 mg/l(32°C)[g]<br>4320 mg/l(25°C)[h] | 1000 mg/l (32°C)[g]<br>896(25°C)[h] | 13 mg/l(25°C)[h] | 3 mg/l(25°C)[h] | 0.4 mg/l (25°C)[h]<br>1.3 mg/l[f] | 2.9 mg/l[f] |
| Log octanol/water partition coefficient | 2.12[i,j] | 3.22[i,j] | 5.2[i,j,k] | 9.2[i,j,k] | 8.73[i,j,k]<br>5.3[f] | 5.8[i,j,k]<br>4.8[f] |

---

a) Patty 1963
b) Weast 1977
c) Fishbein and Albro 1972
d) Verschueren 1977
e) EPA-CHMTADS
f) Hirzy et al. 1978
g) Peakall 1975
h) Determined by Wolfe et al. 1979
i) Calculated as per Leo et al. 1971
j) Calculated by Wolfe et al. 1979
k) Value does not include a correction for the influence of molecular folding because data are not available.

Attachment #2

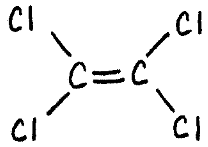
# TETRACHLOROETHENE

File Name: B:PCE
NIOSH# KX3850000

## I. CHEMICAL INFORMATION

Synonyms (10,11):
- Perchloroethylene
- Ethylene Tetrachloride
- Tetrachloroethylene
- Perchloroethene
- Carbon Bichloride
- Percosolve

Structure:



Physical Properties (11 except where noted):
Mol. Wt.: 165.83
Melting Pt.: -22.7 C
Boiling Pt.: 121 C
Vapor Pressure: 19 torr (25 C)(C)
Solubility (20 C): 200 mg/l
Kow: 2.88
Ksc: ~2.9

Uses (3):

PCE is a solvent widely used in the dry cleaning industry, as a degreaser, in veterinary medicine, and in copying machines.

Detection:

PCE is ubiquitous in the environment. It has been detected in finished drinking water, marine and rain water, food, human tissues, the atmosphere, and in marine organisms. (4,11) The PCE level in ambient water is reported to be minimal due to its high volatility (4).

Fate in the Envrironment (11 except where noted):

Volatilization: Volatilization is the main transport process.

Photolysis, Oxidation: Photodissociation and oxidation are not significant, although there can be significant photooxidation in acqueous media in the prescence of sunlight.

Sorption: Probably not important.

Hydrolysis: PCE decomposes slowly in water. Its low solubility and vapor pressure indicate that it is persistent, particularly in deeper soil or GW. Because of low solubility, PCE should not migrate rapidly through soil. (C) Estimated hydrolytic half life 8.8 months at ~25 C. Decomposition is accelerated by the prescence of oxygen. Breakdown products are Trichloroacetic Acid and Hydrogen Chloride.

Bioaccumulation: PCE has the potential to bioaccumulate, with ratios of concentrations in various organs proportional to fat content. No evidence exists for biomagnification in aquatic food chains.

Biotransformation/Biodegradation: Some evidence exists that PCE can be metabolized by mammals to trichloroacetic acid, which in turn can be broken down by microorganisms. (4,11)

PCE will sink and lie in an immiscible layer at the bottom of a water course; it may smother benthic life.

## II. TOXICITY INFORMATION (10 except where noted)

PCE is widely absorbed by all routes (inhalation, oral, dermal). The primary acute effect at low doses is to the CNS - PCE can cause depression, ataxia, unconciousness, respiratory and cardiac arrest. Upon ingestion, it causes irritation of the gastrointestinal tract, which, in turn, causes nausea, vomiting, diarrhea, and bloody stools. Such effects are less severe than those of swallowing similar amounts of other chlorinated hydrocarbons.(3) Higher acute doses can cause renal damage, fatty infiltration and necrosis of the liver. Chronic low level exposure can result in headache, fatigue, somnolence, dizziness, and an intolerance to alcohol. Higher chronic doses can result in damage to the liver, kidneys, and CNS. PCE is not flammable. However, when heated it emits highly toxic chloride fumes. (C)

Irritation Data:
skin rabbit - 810 mg/24 hrs - severe
eye rabbit - 162 mg - mild

Oral LD50:

| | |
|---|---|
| 8850 mg/kg | (rat) |
| 8100 " | (mouse) |

Dermal LD50:
insufficient data

Aquatic LC50 (96 hrs):
100-10 ppm

Mutagenicity:

| | |
|---|---|
| mmo-sat | 50 uL/plate |
| mma-sat | 200 uL/plate |
| dns-hmn:lng | 100 mg/L |
| otr-rat:emb | 97 mmol/L |
| cyt-rat-ihl | 500 ppm |
| hma-mus/sat | 100 ppm |
| spm-mus-ihl | 500 ppm |

Carcinogenicity:

EPA Carcinogen Assessment Group has determined that PCE is a carcinogen based upon several animal studies. CAG estimated daily exposure of 8.0 mg will result in a e-5 excess cancer risk level. (C) NCI found hepatocellular carcinoma in mice. (4) IARC determination: Animal suspected. (3)

Teratogenic Effects:
Insufficient information.

Reproductive Effects:

6 ref. of reproductive effects in rats and mice (route inhalation) - lowest dose effect 300 ppm/7 hrs.

## III. STANDARDS (4 except where noted)

EPA water quality criteria to protect human health:

| | Increased Cancer Risk | | | |
|---|---|---|---|---|
| | 1/ 100,000 | 1,000,000 | 10,000,000 | |
| Ambient Water Concentration | 8.0 | 0.8 | 0.08 | ug/l |
| Consumption of Aquatic Organisms Only | 88.5 | 8.85 | 0.88 | ug/l |

EPA aquatic criterion levels - 310 ug/l 24 hr. average
- 700 " Ceiling

EPA adjusted Acceptable Daily Intake (ADI): 0.085 mg/l (5)

EPA projected upper limit lifetime cancer risk estimates 1/100,000:

| CAG | proposed CAG | NAS | | |
|---|---|---|---|---|
| 10 | - | 35 | ug/l | (5) |

DOHS recommended action level: 4 ppb (17)

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 4 |
| Bioaccumulation | 3 |
| Acute Toxicity | |
| oral LD50: | 0 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 3 |
| Carcinogenicity | 10b |
| Mutagenicity | 10 |

# TOLUENE

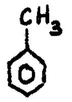
File Name: Toluene
NIOSH #: XS5250000

## I. CHEMICAL INFORMATION

Synonyms: (10)
- Methylbenzene
- Methacide
- Phenylmethane
- Toluol

Structure: (11)

$C_6H\ CH_3$



aromatic hydrocarbon

Physical Properties: (11)

| | | | |
|---|---|---|---|
| Molecular Wt. | 92.13 | Flammable | |
| Melting Point | -95C | Solubility 25C | 534.8mg/L |
| Boiling Point | 110.6C | Kow | 2.69 |
| Vapor Pressure 25C | 28.7torr | Ksc | ~ 2.7 |

Uses: (12,3)

industrial solvent used in paints, varnishes, glues, enamels, lacquers; as thinners for oils, dyes, perfumes; chemical intermediate in synthesis of organic compounds (pronounced fungisitic, antihelminthic; limited bacteriostatic); suspension solvent for navigational instruments, nonclinical thermometer liquid; adhesive solvent in plastic toys, model airplanes; explosives (TNT); detergents.

Detection: (11)

Detected in finished drinking water, industrial effluents, ambient surface waters.

Fate in the Environment: (11,16)

Volatilization - significant transport process for removal from water; halflife is 5.18 hrs
Oxidation - predominant fate in atmosphere; halflife = ~15hrs
Photolysis - not probable
Hydrolysis - not significant
Sorption - Kow indicates may be significant but no data
Bioaccumulation - probably not; solubility >50 mg/L have little aquatic bioaccumulation
Biotransformation/Biodegradation - some species of soil bacteria able to use as sole carbon source (*Pseudomonas desmolytica, Norcardia, Aeruginosa,* & *P. oleovorans*); microbial degradation to acetic and pyruvic acids, primarily through side chain hydroxylation; mammalian degradation to hippuric acid excreted in urine.
BOD = 2.15 g $O_2$/g Toluene; COD = 2.52 g $O_2$/g Toluene (16).

## II. TOXICITY INFORMATION

Harmful effects: (14,16)
Local - irritaion of eyes, respiratory tract, skin
Systemic - central nervous system depression; headache, dizziness, fatigue, muscular weakness, drowsiness, ataxia, skin paresthia, collapse, and coma; liver and kidney effects. Readily absorbed in GI tract; poorly absorbed through skin.
Potentiating over additive effects for certain combinations of Toluene and other chemicals.
Toluene used industrially is seldom pure; usually contains substantial amounts of benzene & other aromatic hydrocarbons
Toxicity rating - 4 (very toxic); probable oral lethal dose (human) 50-500 mg/kg, between 1 teaspoon & 1 oz for 70 kg (150 lb) person (16).

Irritation Data: (10)
eye human 300 ppm
skin rabbit 435 mg, mild 500 mg, moderate
eye rabbit 870 ug mild
eye rabbit 2 mg/24hr severe
eye rabbit 100 mg/30sec rinsed, mild

Toxicity Data: EPA TSCA, (10)
oral rat LD50: 5000 mg/kg
skin rabbit LD50: 12124 mg/kg

Aquatic Toxicity: (10,16)
LC50: 100-10 ppm
LC50: Bluegill (*Lepomis macrochirus*) 17 mg/L/24 hr
" 13 mg/L/96 hr
(95% confidence limit 11-15 mg/L at 21-23C) (16)

Carcinogenicity: (10)
NTP Carcinogenesis study 12/83; no determination

Mutation Data: (10)
EPA Genetic Toxicology Program 1/84
unscheduled DNA synthesis - *Escherichia coli*: 1 pph
unscheduled DNA synthesis-other microorganisms: 1pph/15min cont
cytogenetic analysis - *Saccharomyces cerevisiae*: 2400 umol/tube
DNA damage - rat liver: 30 umol/L
cytogenetic analysis - rat inhalation: 610mg/m /16wk intermit
cytogenetic analysis - rat subcutaneous: 12mg/kg/12d intermit

Reproductive Effects Data: (10)
oral mouse TDlo: 9; 15; 30 gm/kg 6-15d preg
inhalation rat TClo: 1500 mg/m /24hr 1-8d preg
inhalation rat TClo: 1000 mg/m /24hr 7-14d preg
inhalation mouse TClo: 500 mg/m /24hr 6-13d preg
inhalation mouse TClo: 1000 ppm/6hr 2-17d preg

## III. STANDARDS

EPA Priority Pollutant
Permissible Concentration in Water: (14)
To protect human health - 14.3 mg/L

To protect freshwater aquatic life - acute = 17500 ug/L
To protect saltwater aquatic life - acute = 6300 ug/L
chronic = 5000 ug/L
DOHS Action Level - 100 ppb

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 3.5 |
| Bioaccumulation | 3.5 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0 |
| aquatic LD50: | 3 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 10 |

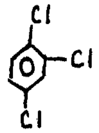
# 1,2,4-TRICHLOROBENZENE

File Name: 124-T
NIOSH #: DC2100000

## I. CHEMICAL INFORMATION

Synonyms: (10)
unsym-Trichlorobenzene
1,2,4-Trichlorobenzol

Structure: (11)



$C_6H_3Cl_3$
aromatic hydrocarbon

Physical Properties: (11)

| | | | |
|---|---|---|---|
| Molecular Wt. | 181.45 | Solubility 25C | 30 mg/L |
| Melting Point | 16.95C | Kow | 4.26 |
| Boiling Point | 213.5C | Ksc | ~ 4.2 |
| Vapor Pressure 25C | .42torr calc. | | |
| " 38.4C | 1 mm Hg | | |

Uses: (12,3)
used in making cellulose acetate, deoderants, disinfectants, dyes, fumigants, lacquers, paints, resins, herbicides; used as a degreaser, and potential insecticide against termites.

Detection: (11)
Detected in drinking water, in waste water effluent, and in the atmosphere.

Fate in the Environment: (11)
Volatilization - at fairly rapid rate; calculated halflife is ~45 minutes when aerated.
Oxidation - suspected in atmosphere; estimated halflife is one to several days
Photolysis - no information
Hydrolysis - probably will not occur
Sorption - Kow indicates substantial process at pollutant concentrations in environmental water; adsorption to organic material.
Bioaccumulation - empirical evidence indicates high potential for bioaccumulation in lipid tissues of living organisms
Biotransformation/Biodegradation - at very slow rate under environmental conditions (unacclimated microorganisms and varying carbon sources).

## III. TOXICITY INFORMATION

Harmful effects: (14,16)
Local - irritating to skin, conjunctiva, and mucous membranes of upper respiratory tract.
Systemic - acute exposure may cause drowsiness, incoordination and unconsciousness; chronic exposure may result in liver, kidney and lung damage indicated by animal experiments.
Toxicity rating - 4(very toxic); probable oral lethal dose (human) 50-500 mg/kg, between 1 teaspoonful & 1 oz for 70kg (150 lb) person (16; Gosselin CTCP 4th ed 1976 II-117).

Irritation Data: (10)
skin rabbit 1950 mg/13 weeks, intermittent moderate

Toxicity Data: (10)
oral rat LD50: 756 mg/kg
oral mouse LD50: 300 mg/kg

Aquatic Toxicity: (10)
LC50: 10-1 ppm

Carcinogenicity: (3)
600 ppm inhaled daily for 6 months caused no hepatomas but not designed as a carcinogenicity study.

Mutagenicity: no information

## III. STANDARDS

EPA Priority Pollutant
Permissible Concentrations in Water: (14)
To protect human health - no criteria developed due to insufficient data.

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 0 |
| Bioaccumulation | 6.5 |
| Acute Toxicity | |
| oral LD50: | 3 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 5 |
| Carcinogenicity | 0-10 |
| Mutatgenicity | 0-10 |

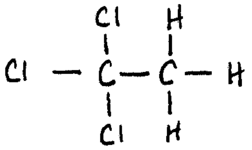
# 1,1,1-TRICHLOROETHANE (TCA)

File Name: B:TCA
NIOSH# KJ2975000

## I. CHEMICAL INFORMATION

Synonyms (10,11):
- Methyl Chloroform
- Chlorotene
- Genklene
- Baltana
- Chlorothene

Structure:



Physical Properties: (11 except where noted):
Mol. Wt.: 133.41
Melt. Pt.: -30.41 C
Boil. Pt.: 74.1 C
Vapor Pressure: 127 torr (25 C) (10)
Solubility: 480-4400 mg/l depending on study
Kow: 2.17 (11) - 2.47 (3)
Ksc: ~2.17-2.47

TCA reacts violently with Acetone, N2O4, both liquid and gaseous oxygen, sodium, and sodium hydroxide; it also reacts vigorously with aluminum, readily corroding aluminum and aluminum alloys. (3)

Uses:

TCA is used almost exlusively as a solvent. Worldwide consumption is about 1 billion lb/yr. Most commercial Methyl Chloroform contains inhibitors to prevent reaction of the solvent with aluminum and aluminum alloys. This reaction produces hydrogen chloride and in confined vessels may produce high pressure. (12) Formerly used for degreening citrus fruits with ethylene gas and fumigating strawberries after harvest. Registered agricultural used have been cancelled. (3)

Detection (11):

1,1,1-TCA is known to be ubiquitous in the environment. It has been detected in the atmosphere, finished drinking water, freshwater, rainwater, seawater, marine sediments, marine organisms, and in surface snow in Alaska.

Fate in the Environment (11):
- Volatilization: Volatilization is the primary transport process.
- Photolysis: Probably not significant in aquatic systems.
- Oxidation: Not significant in aquatic systems.
- Sorption: Probably not important.
- Hydrolysis: Probably occurs too slowly to be a significant fate process. (11) Hydrolyzes at 25 C to Acetic Acid and Hydrochloric Acid. At 10 C and pH 8, vinylidene chloride is the major end product. (3)
- Bioaccumulation: Kow shows a low potential for

bioaccumulation (11). Marine organisms have an accumulation factor of <100 for TCA (3).

Biotransformation/Biodegradation: TCA is metabolized primarily to trichloroethanol and trichloroacetic acid in humans; most is excreted unchanged by the lung. (3)

## II. TOXICITY INFORMATION (10 except where noted)

Acute hazards include changes to exposed tissue and proarrhythmic activity which sensitizes the heart to epinephrine-induced arrhythmias. Narotic in high concentrations. Acute exposure produces a significant toxic effect in the form of a functional depression of the CNS leading to respiratory failure. Chronic exposures can lead to fatty degeneration of the liver and growth depression. (3) Included in EPA TSCA inventory, 1980.

Irritation Data:

eye man - 450 ppm/8 hrs
skin rabbit - 5 gm/12D-I - mild
" " - 500 mg/24 hrs - moderate
eye rabbit - 100 mg - mild
" " - 2 mg/24 hrs - severe

Oral LD50:

750 mg/kg (dog)
5,660 " (rabbit)
9,470 " (guinea pig)
10,300 " (rat)
11,240 " (mouse)

Dermal LD50:

insufficient data

Aquatic LC50 (96 hrs):

100-10 ppm

Toxic effects in humans (GI upset) at 670 mg/kg.

Mutagenicity:

| | |
|---|---|
| mmo-sat | 1 mL/plate |
| mma-sat | 1 mL/plate |
| dnr-esc | 500 mg/L |
| otr-rat:emb | 99 umol/L |
| otr-ham:kdy | 562 mg/L |
| otr-ham:emb | 100 uL/plate |

Included in EPA Genetic Toxicology Program, January 1984.

Carcinogenicity:

Bioassay results negative, IARC determination: animal indefinite. (10) Carcinogenic in prelimary report from NTP (mice studies) - this report is currently being evaluated. (5)

Teratogenic Effects:

No known teratogenic effects. (12)

Reproductive Effects:

3 Inhalation studies have been noted.

## III. STANDARDS

EPA adjusted Acceptable Daily Intake (ADI): 1.0 mg/l (5)

EPA projected upper limit lifetime cancer risk estimates 1/100,000:

| CAG | proposed CAG | NAS |
|---|---|---|
| 217 | - | 168 ug/l (5) |

DOHS recommended action level: 300 ppb (taste and odor threshold); suggested No Adverse Response Level for a 10 kg child 1,000 ppb. (17)

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 4-5 |
| Bioaccumulation | 2-3 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 3 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 10 |

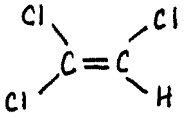
## TRICHLOROETHYLENE (TCE)

File Name: B:TCE
NIOSH# KX4550000

## I. CHEMICAL INFORMATION

Synonyms (10,11):
- Trichloroethene
- Ethylene Trichloride
- Ethinyl Trichloride
- Tri-clene
- Acetylene Trichloride
- Benzinol
- various trade names

Structure:



Physical Properties (11 except where noted):
Moleclular Wt.: 131.29
Melting Pt.: -73 C
Boiling Pt.: 87 C
Vapor Pressure: 57.9 torr at 20 C
Solubility: 1,100 mg/l at 20 C
Kow: 2.29
Ksc: ~2.29

Uses (12):

TCE is a clear, colorless liquid widely used as a degreasing solvent.

Detection (11):

TCE is ubiquitous in the environment. It has been detected in finished drinking water, drinking water supplies, marine water, rain water, food, human tissues, the atmosphere, and in marine organisms.

Fate in the Environment (11 except where noted):

Volatilization: Volatilization is the primary transport process.

Photolysis, Oxidation: Photooxidation occurs in the aquatic environment at a slow rate. Direct oxidation at ambient conditions does not occur in the aquatic or atmospheric environment.(11) TCE is subject to photochemical attack at the unsaturated bond (3).

Sorption: Coarse sediments have little adsorptive capacity for TCE; sediments rich in organic matter have higher adsorptive capacity. Concentrations are similar in sediments and water.

Hydrolysis: TCE is not hydrolyzed by water under normal conditions.

Bioaccumulation: There is some evidence of bioaccumulation but none for biomagnification.

Biotransformation/Biodegradation: There is no information indicating microorganisms exist which can readily degrade TCE. There is some evidence from mammal studies that TCE can be metabolized. The metabolic pathway leads to chlorinated acetic acids, either directly or via chloroethanols. Chlorinated acetic acids are susceptible to further degradation by microorganisms in seawater.

TCE will sink and be found at the bottom of water courses; it dissolves "very very slowly". It may smother benthic life. (3)

## II. TOXICITY INFORMATION (10 except where noted):

TCE is absorbed by all routes (Inh, Oral, Dermal). Its metabolites bioaccumulate, becoming distributed in adipose tissue. (3)

High acute exposures result in anesthesia, narcosis, and death from cardiac failure due to ventricular fibrillation. Lesser effects - mild to severe CNS depression and cardiographic anomalies. (3)

Chronic effects include CNS effects (headaches, insomnia, tremors, neuroasthmatic syndrome, bradycardia, breakdown of Purkinje and basket cells, and mild to severe CNS depression, especially of the peripheral system) and fatty degeneration of the liver. TCE is also reported to be nephrotoxic but data is inconclusive. (3) Included in EPA TSCA inventory, 1980.

Irritation Data:
eye human - 5 ppm
skin rabbit - 500 mg/24 hrs - severe
eye rabbit - 20 mg/24 hrs - severe

Oral LD50:
4920 mg/kg (rat) (3,10)
5860 " (dog) (3)

Oral LD (low):
7 gm/kg (human)

Dermal LD50:
insufficient info

Aquatic LC50:
60 ppm (C)
1000-100 ppm (3)

Mutagenicity:

| | |
|---|---|
| mmo-sat | 100 uL/plate |
| mma-sat | 5 pph/2 H |
| mma-esc | 3300 umol/L |
| mma-smc | 10 gm/L |
| dns-hmn:lng | 100 gm/L |
| dni-hmn:lym | 5 mL/L |
| sce-hmn:lym | 178 mg/L |
| otr-rat:emb | 1100 umol/L |
| dnd-rat:lvr | 100 umol/L |
| slt-mus-ipr | 1 mmol/L |
| dnd-mus:lvr | 100 umol/L |
| dns-mus-orl | 2500 mg/L |
| dns-mus:bmr | 1 mmol/L |
| hma-mus/smc | 400 mg/kg |
| spm-mus-ihl | 100 ppm |

| | |
|---|---|
| otr-ham:emb | 5 mg/L |
| oms-ham:fbr | 1 pph |
| dnd-ham:lym | 1 mmol/L |

Included in EPA Genetic Toxicology Program, January 1984.

Carcinogenicity:

Positive for mice, negative for rats, human suspect (TCE is a listed carcinogen by EPA CAG & NAS. Excess risk of e-4 by daily dose of 560 ug (CAG) or 900 ug (NAS). (C)). IARC determination: Animal positive (3). IARC determinations: Animal Positive, Human Indefinite (10).

Teratogenic Effects:

1 Inhalation study noted (rat).

Reproductive Effects:

5 Inhalation studies noted.

## III. STANDARDS

| | | | |
|---|---|---|---|
| EPA aquatic limits: | 1500 ug/l | 24 hr. average | |
| | 3400 " | at any time | (4) |

EPA projected upper limit lifetime cancer risk estimates 1/100,000:

| CAG | proposed CAG | NAS | |
|---|---|---|---|
| 28 | 18 | 45 | ug/l (5) |

EPA adjusted Acceptable Daily Intake (ADI): 0.26 mg/l (5)

DOHS recommended action level: 5.0 ppb (17)

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 4.5 |
| Bioaccumulation | 2 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 3 |
| Carcinogenicity | 10b |
| Mutagenicity | 10 |

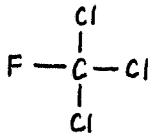
## TRICHLOROFLUOROMETHANE

Flie Name: Freon
NIOSH #: PB6125000

## I. CHEMICAL INFORMATION

Synonyms: (10)
- Fluorotrichloromethane
- Freon 11
- Fluorocarbon 11
- Arcton 9

Structure: (11)



$FCCl_3$

halogenated aliphatic hydrocarbon

Physical Properties: (11)

| | | | |
|---|---|---|---|
| Molecular Wt. | 137.4 | Solubility | 1100 mg/L |
| Melting Point | -111C | Kow | 2.53 |
| Boiling Point | 23.8C | Ksc | ~ 2.5 |
| Vapor Pressure 20C | 667.4torr | | |

Uses: (12)

Used in medicated aerosols.

First aerosol application of fluorocarbons was as insecticide bomb during WW11 to protect troops in tropics against malaria and other vector-borne diseases; Mid-70's used in cosmetic and domestic aerosols, refrigerants, plastic foam agents, and solvents.

1978 EPA prohibitted aerosol use except in medicated aerosols.

Detection: (11)

Detected in surface waters, surface snow in Alaska, seawater, rainwater, and in atmosphere.

Fate in the Environment: (11)

Volatilization - major transport process for removal from aquatic systems
Photolysis - primary fate in stratosphere; lifetime of 10 years; not significant in aquatic systems
Hydrolysis - too slow to be significant process
Oxidation - not significant
Sorption - onto sediments possible but inconclusive
Bioaccumulation - detected at 0.1 to 5.0 ppb (dry wt basis) in various organs of fish and molluscs but not necessarily indicated potential for bioaccumulation; high volatility seems to make persistence in aquatic environment unlikely.

## II. TOXICITY INFORMATION

Harmful effects: (14)

incoherence, tremors, dermatitis, frostbite, cardiac arrythmias, cardiac arrest.

Toxicity Data: EPA TSCA,(10)

| | | | |
|---|---|---|---|
| inhalation | human | TC50: | 50,000 ppm/30 minutes |
| inhalation | rabbit | LC50: | 25 pph/30 minutes |

Aquatic Toxicity: (4)
acute freshwater - as low as 11 ppm
acute saltwater - as low as 12 ppm
chronic saltwater - as low as 6.4 ppm

Carcinogenicity: (10)
NCI Carcinogenesis bioassay completed;
Results - indefinite, rat; negative, mouse

Mutagenicity: no information

## III. STANDARDS

EPA Priority Pollutant
Permissible Concentration in Water: (14)
To protect human health - preferably zero
Additional lifetime cancer risk of 1/100,000 at 1.9 ug/L

EPA criterion level to protect against noncarcinogenic effects is 32.3 mg/L (4)

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 4 |
| Bioaccumulation | 3 |
| Acute Toxicity | |
| oral LD50: | 0-10 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 0-10 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 0-10 |

Note: 1,1,2-Trichloro-1,2,2-trifluoroethane

Insufficient information to rank as individual isomer. Available information as follows: (16)

CAS RN #: 76-13-1

Synonym: Freon-113

Physical Properties:

| | |
|---|---|
| Molecular Wt. | 187.38 |
| Melting Point | -36.4C |
| Boiling Point 760mmHg | 47.7C |
| Density 25C, 4C | 1.5635 |
| Solubility | insoluble in water, sol in alcohol |
| Kow (per DOHS) | 1.65 |

Volatile, Colorless, Nearly Odorless

Toxicity Information:

Harmful effects - inhalation produces central nervous system effects; reversible tissue changes when exposure discontinued.

oral rats LDlo: 45 mg/kg
inhalation human TClo: 4500 ppm

Wistar rats exposed to 12000 ppm of Freon-113, 2 hr/day, 5 days/wk, duration 730 days, tumors 1/6 fibrangiosarcoma (Searle. Chem Carcinogens 1976 158)

Freon-113 investigated for action on pulmaonary surfactant in rats. In vitro ventilation of rat lungs with vapors produced alveolar instability & atelectasis. It can dissolve & displace lipid portion of alveolar surfactant causing alveolar instability.
(Alarie et al. Toxicol Appl Pharmacol, 31 (2): 223-242, 1975)

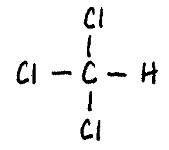
# TRICHLOROMETHANE

File Name: TCHM
NIOSH #: FS9100000

## I. CHEMICAL INFORMATION

Synonyms: (10)
- Chloroform
- TCM
- Trichloroform
- Methyl trichloride

Structure: (11)



$CHCl_3$

halogenated aliphatic hydrocarbon

Physical Properties: (11)

| | | | | |
|---|---|---|---|---|
| Molecular Wt | 119.38 | Volatile | | |
| Melting Point | -63.5C | Solubility | | 8200 mg/L |
| Boiling Point | 61.7C | | 25C | 1ml/200ml |
| Vapor Pressure 20C | 150.0torr | Kow | | 1.97 |
| " 10.4C | 100 mmHg | Ksc | ~ | 2 |

Uses: (3)

used as a solvent, refrigerant; in synthesis of chlorodifluormethane; as insecticidal grain fumigant; in drugs and cosmetics; in extraction and purification of antibiotics; as anesthetic.

Detection: (11)

Ubiquitous in environment; detected in finished drinking water, marine waters and sediments, rainwater, waste water effluent, in food residues, and in air.

Fate in the Environment: (11)

Volatilization - major transport process from aquatic systems; experimental halflife is 20-25 minutes

Photolysis - not significant

Hydrolysis - not significant; minimum halflife is 3500 yr, maximum halflife is 15 months

Oxidation - not significant; lifetime of 0.19-0.32 yrs

Sorption - probably not significant; coarse gravels had little adsorptive capacity whereas sediments rich in organic detritus had much higher adsorptive capacity; No clear evidence of selective concentration in sediments.

Bioaccumulation - weak to moderate; no evidence of biomagnification in marine food chain

Biotransformation/Biodegradation - no specific information; should be degradable by biological sewage treatment; in the sea many invertebrates metabolize halogens.

Other Reactions - found in finished drinking water due to haloform reaction.

## II. TOXICITY INFORMATION

Harmful effects: (14,16)

Local - may cause burns if prolonged skin contact

Systemic - potent anesthetic at high concentrations; exposure causes lassitude, digestive disturbance, dizziness, mental dullness, and coma; liver damage more characteristic than CNS depression or renal injury. Primary toxic response at lower levels of exposure is hepatotoxicity leading to fatty liver & centrilobular necrosis. Effects on liver & kidneys exaggerated by ingestion of alcohol.

Death from use as anesthetic due to liver damage & cardiac arrest.

Toxicity rating - 3 (moderately toxic); probable oral lethal dose (human) 0.5-5 g/kg; between 1 oz & 1 pt (or 1 lb) for 70 kg (150 lb) person; mean lethal dose probably lies near 1 fluid oz (16; Gosselin. CTCP 4th ed 1976 II-110).

Irritation Data: (10)

| | | |
|---|---|---|
| skin | rabbit | 10 mg/24hr open, mild |
| eye | rabbit | 148 mg |

Toxicity Data: EPA TSCA, (10.3,16)

| | | | | |
|---|---|---|---|---|
| oral | human | LDlo: | 140 mg/kg | |
| oral | rat | LD50: | 800 mg/kg | |
| oral | mouse | LD50: | 36 mg/kg | |
| oral | rabbit | LDlo: | 500 mg/kg | |
| oral | dog | LDlo: | 1000 mg/kg | |
| oral | rat | LD50: | 450 mg/kg | |
| oral | rat | LD50: | 300 mg/kg | |
| oral | rat | LDlo: | 70 gm/kg/78wks | intermit, neoplasm |
| oral | rat | TD: | 98 gm/kg/78wks | intermit, neoplasm |
| oral | mouse | TD: | 18 gm/kg/17wks | intermit, neoplasm |

Aquatic Toxicity: (10)

LC50: 100-10 ppm

Carcinogenicity: (10,8,16)

IARC Determination - animal positive (mouse, rat)
human suspect
animal suspect

NCI Carcinogenesis bioassay completed;
Results - positive (mouse, rat)

Hepatocellular carcinoma in mice statistically significant(16)
Renal tumors in rats (8).

Tumorigenic Data: (10,16)

| | | | | |
|---|---|---|---|---|
| oral | rat | TDlo: | 70 gm/kg/78wk | intermit(urogenital/endocrine) |
| oral | mouse | TDlo: | 127 gm/kg/92wk | intermit(liver) |
| oral | rat | TD: | 98 gm/kg/78wk | intermit(urogenital,endocrine) |
| oral | mouse | TD: | 18 gm/kg/17wk | intermit(liver) |
| oral | rat | TD: | 7020 mg/kg/78wk | intermit(liver,urogenital) |

Mutagenicity: (10)

EPA Genetic Toxicology Program 1/84

mutation in microorganism - *Salmonella typhimurium*: 20 ug/plate

microsomal mutagenicity assay - *S. typhimurium*: 20 ug/plate

DNA repair - *Escherichia coli*: 500 mg/L

cytogenic analysis - *Saccharomyces cerevisiae*: 5 mmol/tube

oncogenic transformation - hamster kidney: 4430 mg/L

DNA damage - mammalian lymphocyte: 1 mmol/L

Reproductive Effects Data: (10)

oral rat TDlo: 1260 mg/kg 6-15 days pregnant

inhalation rat TClo: 30; 100; and 300 ppm/7hr 6-15 days pg

oral mouse TDlo: 2177 mg/kg (3wk male/3wk pre-7days post)

oral mouse TDlo: 2115 mg/kg (3wk male/3wk pre-5days post)

oral rabbit TDlo: 260 mg/kg 6-18 days pregnant

Teratogenicity: (7)

Embryotoxic

## III. STANDARDS

EPA Priority Pollutant

Superfund Hazardous Substance List (14)

Permissible Concentration in Water: (14)

To protect human health - preferably zero

Additional lifetime cancer risk of 1/100,000 at 1.9 ug/L

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 6 |
| Bioaccumulation | 2 |
| Acute Toxicity | |
| oral LD50: | 5 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 3 |
| Carcinogenicity | 10a |
| Mutagenicity | 10 |

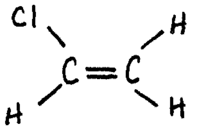
# VINYL CHLORIDE

File Name: B:VC
NIOSH# KU9625000

## I. CHEMICAL INFORMATION

Synonyms (11):
- Chloroethene
- Monochloroethylene
- Monovinylchloride
- MVC
- Chloroethylene

Structure:



Physical Properties (11):
Mol. Wt.: 62.50
Melting Pt.: -153.8 C
Boiling Pt.: -13.37 C
Vapor Pressure: 2,660 torr (25 C)

Solubility: 1.1-60 mg/l depending on study
Kow: 0.60
Ksc: ~0.6

Uses (4):

Vinyl Chloride is used in the manufacture of polyvinyl chloride (PVC), which in turn is used to make assorted plastics.

Detection (11):

Vinyl Chloride has been detected in finished drinking water by the National Organics Reconnaissance Survey (NORS). It has been detected in the atmosphere and in industrial waterborne discharges.

Fate in the Environment (11 except where noted):
- Volatilization: Volatilization is the primary transport process.
- Photolysis: Not a significant fate process. No photolysis occurs at wavelengths greater than 300 nm.
- Sorption: Probably not a significant transport process.
- Oxidation: Oxidation in the aquatic environment is probably not significant.
- Hydrolysis: Hydrolysis from pH 4.3-9.4 is not an important pathway for removal from water.
- Bioaccumulation: There is very little potential for bioaccumulation.
- Biotransformation/Biodegradation: Vinyl Chloride is resistant to microbial degradation.

Vinyl Chloride should not remain in an aquatic ecosystem under normal conditions. (4) VC decomposes rapidly in the prescence of Acetone or Hydrogen Peroxide and UV light. (11) Alkali metal salts increase solubility. (4)

## II. TOXICITY INFORMATION (10 except where noted)

Problems associated with Vinyl Chloride exposure include Raynaud's Syndrome, dermatitis, scleroderma, thyroid insufficiency, hepatomegaly, acro-osteolysis of the distal phalanges, functional disturbances of the CNS withadrenergic sensory polyneuritis, thrombocytopenia, splenomegaly, liver malfunction with marked fibrosis in the portal areas, and pulmonary insufficiency with restrictive changes in the lungs. (4)

Irritation Data:
insufficient information

Oral LD50:
500 mg/kg (rat)

Dermal LD50:
insufficient information

Aquatic LC50 (96 hrs):
100-10 ppm

Mutagenicity:

| | |
|---|---|
| mmo-sat | 2,000 ppm/48 H |
| mma-sat | 20 pph/4 H |
| mma-esc | 10,600 umol/L |
| dnr-esc | 100 ug/plate |
| sln-dmg-ihl | 1 pph |
| sln-dmg-orl | 850 ppm |
| mma-smc | 25,000 ppm |
| mrc-smc | 48 mmol/L/3 H |
| mmo-ssp | 130 ppm |
| mma-ssp | 16 mmol/L/30 M |
| mrc-ssp | 48 mmol/L |
| cyt-man-unk | 25 ppm/10 Y |
| cyt-hmn:hla | 10 mmol/L |
| otr-rat-ihl | 2,000 ppm/14 W-I |
| dnd-rat-orl | 18 gm/kg/2 Y-C |
| oms-rat:lvr | 1 nmol |
| cyt-rat-ihl | 150 ug/m3/14 W-C |
| hma-rat/smc | 1 pph/24 H-C |
| mnt-mus-ihl | 5 pph/4 H |
| hma-mus/ssp | 700 mg/kg |
| hma-mus/smc | 700 mg/kg |
| mma-ham:lng | 20 pph/5 H |
| cyt-ham-ihl | 12,500 ppm/6 H |
| cyt-ham-mul | 600 mg/kg |
| sce-ham-ihl | 12,500 ppm/6 H |
| msc-ham:ovr | 10 pph |

Carcinogenicity:
At first found to cause liver angiosarcoma in animals and humans (3,4), it is now known to cause brain cancers and lung cancers in humans working with it and is a multipotent carcinogen based on animal studies (3). IARC determination: Human and

animal positive; reported in the NTP *3rd Annual Report on Carcinogens*, 1982 (10).

Reproductive Effects:
8 ref. of reproductive effects in rats, mice, and humans (route inhalation) - lowest dose effect for humans 30 mg/m3.

Teratogenic Effects:
Statistically significant excess occurances of minor skeletal abnormalities in rats, rabbits, and mice whose mothers were exposed 7 hours daily to concentrations of Vinyl Chloride ranging from 50 to 2,500 ppm (mice and rats were exposed from days 6 to 15 of pregnancy, rabbits from days 6 to 18). At high concentrations there was evidence of fetal death in all 3 species. Significantly greater numbers of congenital malformations of the CNS, upper alimentary tract, genital organs, and feet were reported in 3 small communities in which Vinyl Chloride polymerization plants are located. (4)

## III. STANDARDS

EPA water quality criteria to protect human health (4):

| Standard | Increased Cancer Risk (ug/l) | | |
|---|---|---|---|
| | 1/ 100,000 | 1,000,000 | 10,000,000 |
| Ambient Water Concentration | 20 | 2.0 | 0.2 |
| Consumption of Aquatic Organisms Only | 5,246 | 525 | 52.5 |

EPA projected upper limit lifetime cancer risk estimates 1/100,000:

| CAG | proposed CAG | NAS |
|---|---|---|
| 20 | 0.15 | 10 ug/l (5) |

EPA adjusted Acceptable Daily Intake (ADI): 0.06 mg/l (5)

DOHS recommended action level: 2.00 ppb (17)

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 10 |
| Bioaccumulation | 0 |
| Acute Toxicity | |
| oral LD50: | 3 |
| dermal LD50: | 0-10 |
| aquatic LC50: | 3 |
| Carcinogenicity | 10c |
| Mutagenicity | 10 |

# XYLENE

File Name: Xylene
NIOSH #: Xylene ZE2100000
o-Xylene ZE2450000 m-Xylene ZE2275000 p-Xylene ZE2625000

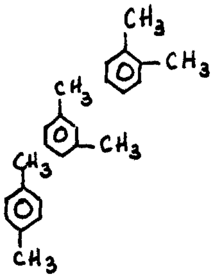
## I. CHEMICAL INFORMATION

Synonyms: (10)
Dimethylbenzene
Xylol

Structure: (12)
o-Xylene $1,2\text{-}C_6H_4(CH_3)_2$

m-Xylene $1,3\text{-}C_6H_4(CH_3)_2$

p-Xylene $1,4\text{-}C_6H_4(CH\ )_2$



Physical Properties: (12)

| Flammable | o | m | p |
|---|---|---|---|
| Molecular Wt. | 106.2 | 106.2 | 106.2 |
| Melting Point | -25.18C | -47.9C | 13.26C |
| Boiling Point | 144.4 | 139.10 | 138.3 |
| Vapor Pressure 20C | 5mm | 6mm | 6.5mm |
| Solubility | 175mg/L20C | no info | 198mg/L25C |
| Kow | 2.77 | 3.20 | 3.15 |
| Ksc | ~ 2.7 | ~ 3.2 | ~ 3.1 |

Uses: (8)

Used in the manufacture of quartz crystal oscillators, epoxy resins; as thinners, solvents for ink, rubber, gums, adhesives and lacquers, paint removers, and in paper coating; as solvent and emulsifiers in agricultural products, fuel components; as chemical intermediates to replace benzene; pharmaceuticals.

o-Xylene also used as raw material for production of plasticizers, alkyd resins, glass-enforced polyesters;

m-Xylene also used in organic synthesis of Isophthalic acid, insecticides, and aviation fuel;

p-Xylene also used for synthesis of tetraphthalic acid.

Detection: (16)

Release of xylenes into the environment each year is estimated to be nearly 410 million kg.

Fate in the Environment: (15)

Volatilization - calculated halflife is 5.61 hrs based on evaporative loss for a water depth of 1m at 25C

Oxidation - o-Xylene cooxidation to o-Toluic acid by Nocardia using hexadecane and by Pseudomonas using hexane as growth substrate; p-Xylene cooxidation to p-Toluic acid by Nocardia using hexadecane as growth substrate.

Biodegradation - o,m,p isomers biodegrade 100% after 192 hrs at 13C incubation with natural flora in Groundwater; some species of microorganisms use m- and p-xylene as sole energy source; m-Xylene does not biodegrade well, persistent (3).

No other information re: other environmental fate processes.

## II. TOXICITY INFORMATION (EPA TSCA)

Harmful effects: (14,16)

Local - irritaion to eyes, nose, and throat; dermatitis; aspiration of a few milliliters of liquid xylene may cause chemical pneumonitis, pulmonary edema, and hemmorhage; repeated exposure of the eyes to high vapor concentrations may cause reversible eye damage.

Systemic - acute vapor exposure may cause CNS depression and minor reversible liver and kidney effects; at high vapor concentrations, dizziness, ataxia, drowsiness, unconsciousness, anorexia, nausea, vomiting & abdominal pain, pulmonary edema.

Xylenes have been reported to cross the human placenta (16). In humans absorbed mainly through mucous membranes & pulmonary systems; absorbed readily via oral, dermal (broken & intact skin); translocated through vascular system; excreted by humans in urine as methylhippuric acids, small portion as xylenol. Identified in mother's milk. (16)

Commercial xylene is a mixture of 3 isomers - o,m,p - with m (meta) usually principal component.

Toxicity rating - 4 (very toxic); probable oral lethal dose (human) 50-500 mg/kg, between 1 teaspoon & 1 oz for 70 kg (150 lb) person (16).

A. Xylene (10,16)

Irritation Data:

| | | | |
|---|---|---|---|
| eye | human | 200 ppm | |
| skin | rabbit | 100% moderate, | 500 mg/24 hr, moderate |
| eye | rabbit | 87 mg mild; | 5 mg/24 hr, severe |

Toxicity Data:

| | | | |
|---|---|---|---|
| oral | rat | LD50: | 4300 mg/kg |
| oral | rat | LDlo: | 7 mg/kg (16) |

Aquatic Toxicity:

LC50: 100-10 ppm

Carcinogenicity:

NTP Carcinogenesis Study completed 12/83;
no determination status.

Mutation Data:

EPA Genetic Toxicology Program 1/84

cytogenetic analysis - *Saccharomyces cerevisiae*: 1 mmol/tube

Reproductive Effects Data:
inhalation rat TClo: 1000 mg/m /24 hr (9-14 days preg)
oral mouse TClo: 20.6 mg/kg (6-15 days preg)
oral mouse TDlo: 31 mg/kg (6-15 days preg)
inhalation mouse TClo: 2000 and 4000 ppm/6 hr 6-12d preg

### B. o-Xylene (10)

Toxicity Data:
oral rat LDlo: 5000 mg/kg

Reproductive Effects Data:
inhalation rat TClo: 150; 1500; 3000 mg/m /24 hr 7-14d preg

### C. m-Xylene (10)

Irritation Data:
skin rabbit 10 ug/24 hr open, severe

Toxicity Data:
oral rat LD50: 5000 mg/kg
skin rabbit LD50: 14100 mg/kg

Reproductive Effects Data:
inhalation rat TClo: 3000 mg/m /24 hr 7-14d preg
oral mouse TDlo: 12 mg/kg 12-15d preg
oral mouse TDlo: 30 mg/kg 6-15d preg

### C. p-Xylene

Toxicity Data:
oral rat LD50: 5000 mg/kg

Reproductive Effects Data:
inhalation rat TClo: 3000 mg/m /24 hr 9-10d preg
inhalation rat TClo: 150 mg/m /24 hr 7-14d preg
inhalation rat TClo: 3000 mg/m /24 hr 7-14d preg
oral mouse TDlo: 12 mg/kg 12-15d preg

## III. STANDARDS

Not EPA Priority Pollutant
Permissible Concentration in Water: (14)
No criteria set
Suggested ambient goal 6000 ug/L based on health effects
Recommended Drinking Water Limits - 2 ppm (3)
DOHS Action Level - 620 ppb

## IV. RANKING

| | |
|---|---|
| Soil Sorption | 1.0-3.5 |
| Bioaccumulation | 3.5-4.0 |
| Acute Toxicity | |
| oral LD50: | 1 |
| dermal LD50: | 0 |
| aquatic LC50: | 3 |
| Carcinogenicity | 0-10 |
| Mutagenicity | 3 |

# III. MUTAGENICITY DATA ABBREVIATIONS

# MUTAGENICITY DATA ABBREVIATIONS

taken from Registry of Toxic Effects of Chemical Substances,
1981-82 Edition, Volume 1, June 1983

Mutation Test System. A number of test systems are used to detect genetic alterations caused by chemical substances. Those systems specifically cited in the Registry are listed below; others found in the literature have been grouped together under the general term "other mutation test system" (oms). Each specific test system is identified by the 3-letter code shown in parentheses. For additional information about mutation tests, the reader may wish to consult the Handbook of Mutagenicity Test Procedures, edited by B. J. Kilbey, M. Legator, W. Nichols, and C. Ramel (Amsterdam: Elsevier North-Holland Biomedical Press, 1977).

(1) Mutation in Microorganisms (mmo) - System utilizes the detection of heritable genetic alterations in microorganisms which have been exposed directly to the chemical substance.

(2) Microsomal Mutagenicity Assay (mma) - System utilizes an in vitro technique which allows enzymatic activation of promutagens in the presence of an indicator organism in which induced mutation frequencies are determined.

(3) Micronucleus Test (mnt) - System utilizes the fact that chromosomes or chromosome fragments may not be incorporated into one or the other of the daughter nuclei during cell division.

(4) Specific Locus Test (slt) - System utilizes a method for detecting and measuring rates of mutation at any or all of several recessive loci.

(5) DNA Damage (dnd) - System detects the damage to DNA strands including strand breaks, crosslinks, and other abnormalities.

(6) DNA Repair (dnr) - System utilizes methods of monitoring DNA repair as a function of induced genetic damage.

(7) Unscheduled DNA Synthesis (dns) - System detects the synthesis of DNA during usually non-synthetic phases.

(8) DNA Inhibition (dni) - System detects damage that inhibits the synthesis of DNA.

(9) Gene Conversion and Mitotic Recombination (mrc) - System utilizes unequal recovery of genetic markers in the region of the exchange during genetic recombination.

(10) Cytogenetic Analysis (cyt) - System utilizes cultured cells or cell lines to assay for chromosomal aberrations following the administration of chemical substances.

(11) Sister Chromatid Exchange (sce) - System detects the interchange of DNA in cytological preparations of metaphase chromosomes between replication products at apparently homologous loci.

(12) Sex Chromosome Loss and Nondisjunction (sln) - System measures the nonseparation of homologous chromosomes at meiosis and mitosis.

(13) Dominant Lethal Test (dlt) - A dominant lethal is a genetic change in a gamete that kills the zygote produced by that gamete. In mammals, the dominant lethal test measures the reduction of litter size. In insects, it measures the number of unhatched eggs.

(14) Mutation in Mammalian Somatic Cells (msc) - System utilizes the induction and isolation of mutants in cultured mammalian cells by identification of the gene change.

(15) Host-Mediated Assay (hma) - System uses two separate species, generally mammalian and bacterial, to detect heritable genetic alteration caused by metabolic conversion of chemical substances administered to host mammalian species in the bacterial indicator species.

(16) Sperm Morphology (spm) - System measures the departure from normal in the appearance of sperm.

(17) Heritable Translocation Test (trn) - Test measures the transmissibility of induced translocations to subsequent generations. In mammals, the test uses sterility and reduced fertility in the progeny of the treated parent. In addition, cytological analysis of the F1 progeny or subsequent progeny of the treated parent is carried out to prove the existence of the induced translocation. In Drosophila, heritable translocations are detected genetically using easily distinguishable phenotypic markers, and these translocations can be verified with cytogenetic techniques.

(18) Oncogenic Transformation (otr) - System utilizes morphological criteria to detect cytological differences between normal and transformed tumorigenic cells.

(19) Phage Inhibition Capacity (pic) - System utilizes a lysogenic virus to detect a change in the genetic characteristics by the transformation of the virus from noninfectious to infectious.

(20) Body Fluid Assay (bfa) - System uses two separate species, usually mammalian and bacterial. Test substance is first administered to host, from whom body fluid (e.g., blood or urine) is subsequently taken. This body fluid is then tested in vitro, and mutations are measured in the bacterial species.

RTECS Mutagenicity Abbrevations Con't

Those test species that are peculiar to mutation data cited in the Registry are designated by the 3-letter codes shown below. Other species are listed in Table II.

| | Code | Species |
|---|---|---|
| Bacteria: | bcs | Bacillus subtilis |
| | esc | Escherichia coli |
| | hmi | Haemophilus influenzae |
| | klp | Klebsiella pneumoniae |
| | sat | Salmonella typhimurium |
| | srm | Serratia marcescens |
| Molds: | asn | Aspergillus nidulans |
| | nsc | Neurospora crassa |
| Yeasts: | smc | Saccharomyces cerevisiae |
| | ssp | Schizosaccharomyces pombe |
| Protozoa: | clr | Chlamydomonas reinhardi |
| | eug | Euglena gracilis |
| | omi | other microorganisms |
| Insects: | dmg | Drosophila melanogaster |
| | dpo | Drosophila pseudo-obscura |
| | grh | grasshopper |
| | slw | silkworm |
| | oin | other insects |
| Fish: | sal | salmon |
| | ofs | other fish |

If the test organism is a cell type from a mammalian species (see Table II), the parent mammalian species is reported, followed by a colon and the cell type designation. For example, human leukocytes are coded "hmn:leu." The various cell types currently cited in the Registry are listed below.

| Designation | Cell Type |
|---|---|
| ast | Ascites tumor |
| bmr | bone marrow |
| emb | embryo |
| fbr | fibroblast |
| hla | HeLa cell |
| kdy | kidney |
| leu | leukocyte |
| lng | lung |
| lvr | liver |
| lym | lymphocyte |
| mmr | mammary gland |
| ovr | ovary |
| spr | sperm |
| tes | testis |
| oth | other cell types not listed above |

# IV. REFERENCES

# REFERENCES

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